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Supporting Information

Synthesis of Cyclopentaquinolinone and Cyclopentapyridinone from *ortho-alkynyl-N-arylaldehyde via* Superbase-promoted C-N, C-O and C-C Bonds Formation

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X-Ray Crystallographic Studies

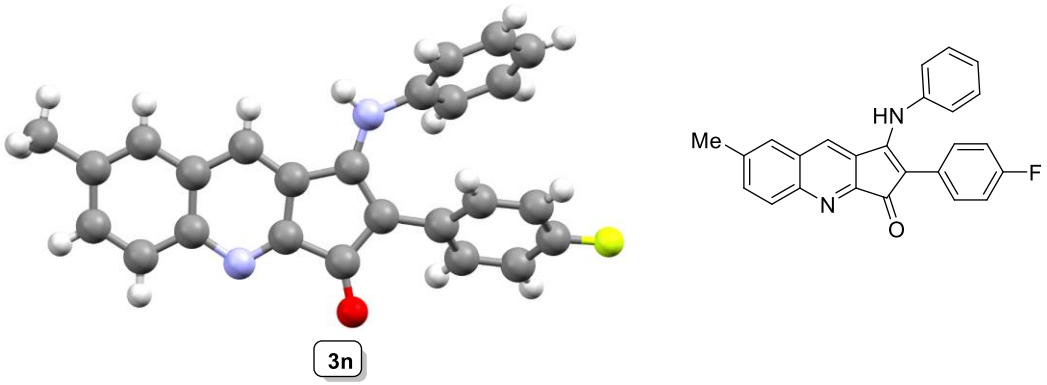


Figure I. ORTEP structure of compound **3n.**

The crystal of **3n** of suitable quality was obtained from MeOH/$CHCl_3$. The compound **3n** crystallized in Monoclinic crystal system with space group *P 1 21 1*. The single-crystal X-ray data were collected on an Oxford X Calibur CCD diffractometer using graphite monochromated Mo Kα radiation (λ = 0.71073 Å). The structures was solved using SIR-92 and refined by full matrix least square technique on F^2 using the SHELXL-97[1-4] program within the WinGX v 1.80.05 software package. In **3n** hydrogens are mixed and all non-hydrogen atoms were refined anisotropically. Atomic coordinates, bond lengths, bond angles, and thermal parameters for compound **3n** have been deposited at the Cambridge Crystallographic Data Centre. CCDC deposit number for **3n** is 1972359.

Table I. Crystallographic data and structure refinement for compounds **3n**

Formula weight	398.42
Temperature	298 K
Wavelength	0.71073 Å
Space group	P 1 21 1
A	6.1550(5) Å
B	15.2830(11) Å
C	10.6069(9) Å
α	90°
β	94.491(6) °
γ	90°
Volume	994.69(14)Å^3
Z	2
Density (calculated)	1.330 g/cm^3
Absorption coefficient	0.091mm^{-1}
F(000)	416.0
Crystal size	0.20 x 0.18 x 0.16 mm^3
Theta max for data collection	26.367°

$^{a}R = \sum(\| Fo | - | Fc \|) / \sum | Fo |$; $^{b}wR = \{\sum[w(F_o^2 - F_c^2)^2] / \sum[w(F_o^2)^2]\}^{1/2}$

References:

1. CrysAlisPro, Agilent Technologies, Version 1.171.34.49, **2011**.

2. Sheldrick, G. M., *ActaCryst*. **2008**, *A64*, 112.

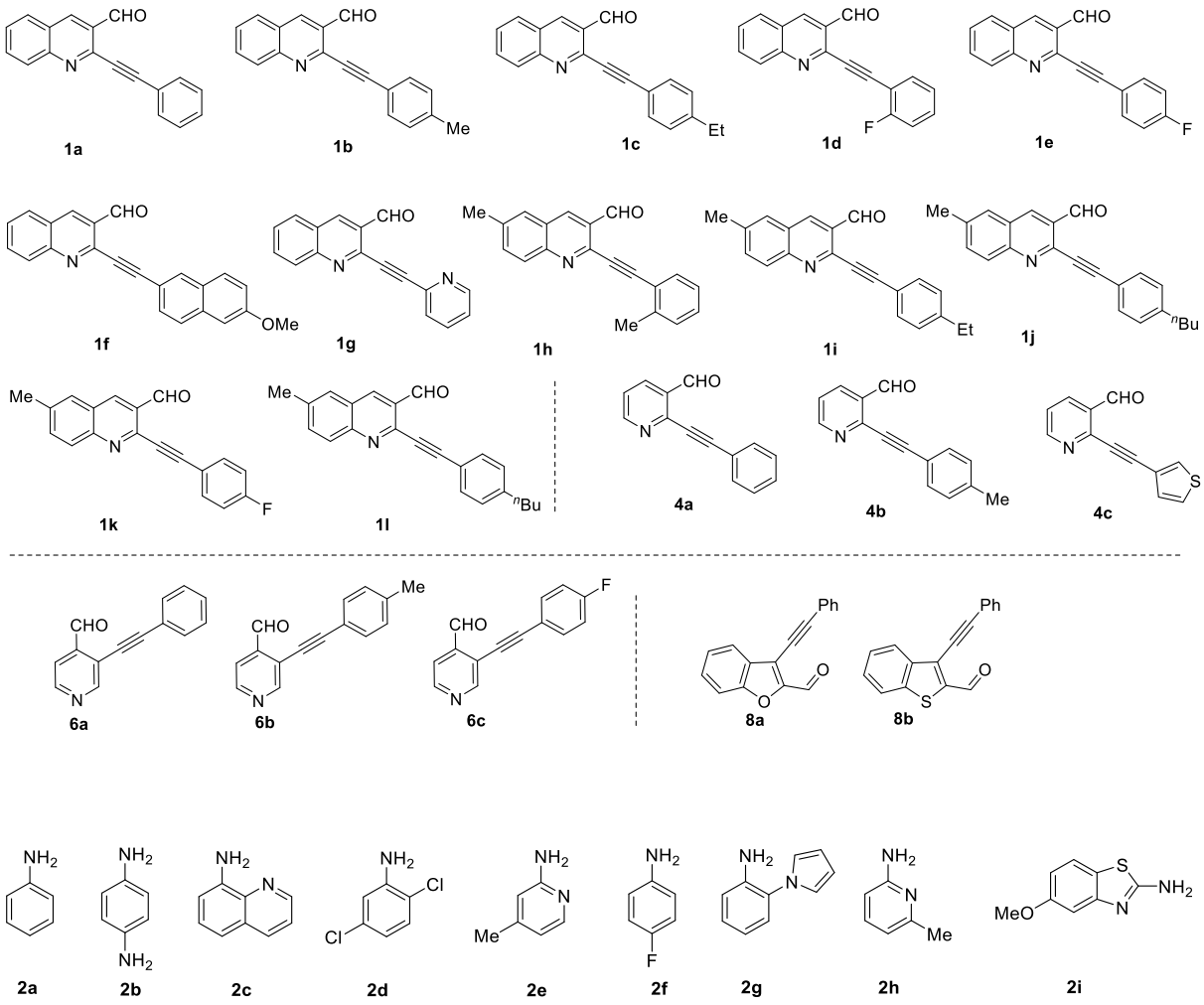
3. Farrugia, L. J. WinGX Version 1.80.05, An integrated system of Windows Programs for the Solution, Refinement and Analysis of Single Crystal X-Ray Diffraction Data*;* Department of Chemistry, University of Glasgow,**1997-2009**.

4. (a) Foresman, J. B.; Frisch, A. E. *Exploring Chemistry with Electronic Structure Methods*; Gaussian, Inc.: Pittsburgh, PA. **1995**. (b) Hehre, W. J., Radom, L., Schleyer, P. V. R.; Pople, J. A. *Ab Initio Molecular Orbital Theory*; Wiley: New York, **1985**.

General Experimental

General Information and Method. All the reactions were performed in an oven-dried Schlenk flask under an argon atmosphere. Column chromatography was performed using silica gel (mesh 100-200). TLC analysis was performed on commercially prepared 60 F_{254} silica gel plates. Visualization of spots on TLC plate was accomplished with UV light (254 nm) and staining over I_2 chamber. ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) spectra were recorded in $CDCl_3$ and $(CD_3)_2SO$. Chemical shifts for carbons are reported in ppm from tetramethylsilane and are referenced to the carbon resonance of the solvent. Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, dd = doublet of doublet, br s = broad singlet), coupling constants in Hertz, and integration. High-resolution mass spectra were recorded with q−TOF electrospray mass spectrometer. All purchased chemicals were used as received. All melting points are uncorrected.

General Procedure for the Synthesis of Starting Substrate 1, 4, 6, 8: To a solution of substituted 2-haloaldehyde (0.5 mmol) in MeCN (5 mL), 3 mol% of $Pd(PPh_3)_2Cl_2$ was added. The reaction vial was then sealed and flushed with nitrogen. Then, 1.5 equiv of Et_3N and 0.51 mmol of alkyne were added to the reaction mixture. The reaction was then stirred at 70 °C until TLC revealed complete conversion of the starting material. The reaction mixture was then allowed to cool, was diluted with H_2O, and was extracted with EtOAc (3 × 10 mL). The combined organic layers were dried over Na_2SO_4, concentrated under vacuum, and purified by column chromatography using 100−200 mesh size silica gels (hexane: ethyl acetate) to afford the corresponding product. The structure and purity of known starting materials **1, 4, 6, 8** were confirmed by comparison of their physical and NMR-spectral data (^{1}H NMR and ^{13}C NMR) with those reported in the literature.[1]



General experimental procedure for the synthesis of cyclopenta[b]quinolin-3-one, cyclopenta[b]pyridin-7-one 3, 5, 7, 9: To a solution of *ortho*-alkynylaldehyde **1** (0.5 mmol), amine **2** (0.5 mmol) in DMSO (2.0 mL), 2.0 equiv of KOH was added. The reaction was then stirred at 100 ^{o}C temperature until TLC revealed a complete conversion of the starting material. The reaction mixture was then allowed to cool, was diluted with H_2O, and finally extracted with EtOAc (3 × 10 mL). The combined organic layers were dried over Na_2SO_4, concentrated under vacuum, and purified by column chromatography using 100−200 mesh sized silica gel (hexane: ethyl acetate) to afford the corresponding product.

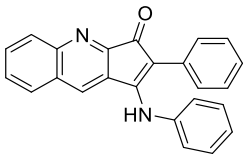
References

1 (a) R. Kumar, A. Chandra, B. A. Mir, and G. Shukla, *J. Org. Chem.*, 2019, **84**,

10710−10723. (b) K. Mishra, J. B. Singh, T. Gupta and R. M. Singh, *Org. Chem. Front.*, 2017, **4**, 1926–1930. (c) A. K. Verma, D. Choudhary, R. K. Saunthwal, V. Rustagi, M. Patel, and R. K. Tiwari, *J. Org. Chem.*, 2013, **78**, 6657−6669. (d) A. K. Verma, V. Rustagi, T. Aggarwal, and A. P. Singh, *J. Org. Chem.*, 2010, **75**, 7691–7703. (e) N. Sharma, M. Asthana, D. Nandini, R. P. Singh, R. M. Singh, *Tetrahedron*, 2013, **69**, 1822–1829. (f) V. Rustagi, R. Tiwari, and A. K. Verma, *Eur. J. Org. Chem.*, 2012, 4590–4602. (g) S., T. Aggarwal, N. Shibata, and A. K. Verma, *Chem. Eur. J.* 2019, **25**, 16063 – 16067. (h) P. Kumar, T. Aggarwal, and A. K. Verma, *J. Org. Chem.*, 2017, **82**, 6388−6397. (h) M. Asthana, J. B. Singh, R. M. Singh, *Tetrahedron Lett.*, 2016, **57**, 615–618. (i) S. Kumar, C. Cruz, S. Pal, R. K. Saunthwal, R. K. Tiwari, E. Juaristi, and A. K. Verma, *J. Org. Chem*. 2015, **80**, 10548–10560

Copies of ^{1}H and ^{13}C NMR

^{1}H NMR



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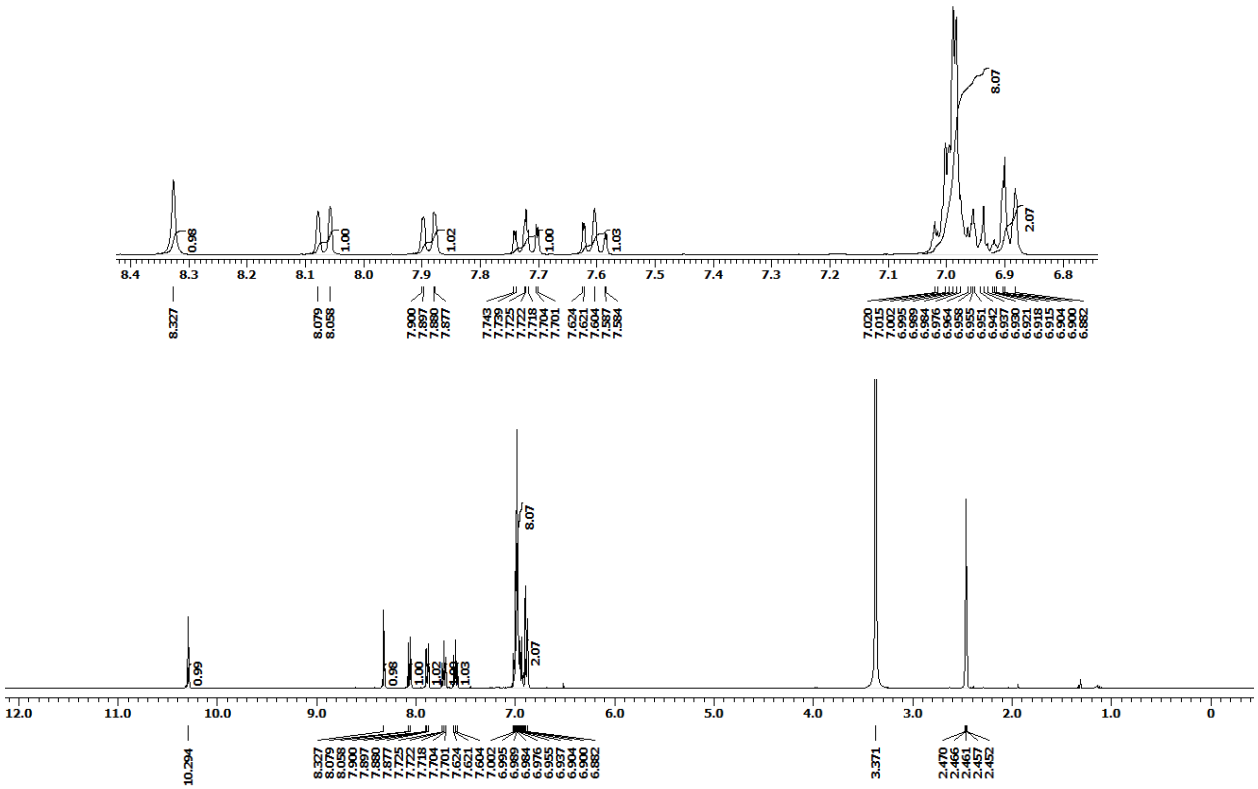
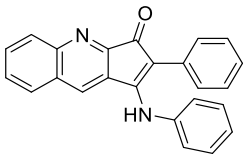


^{13}C NMR



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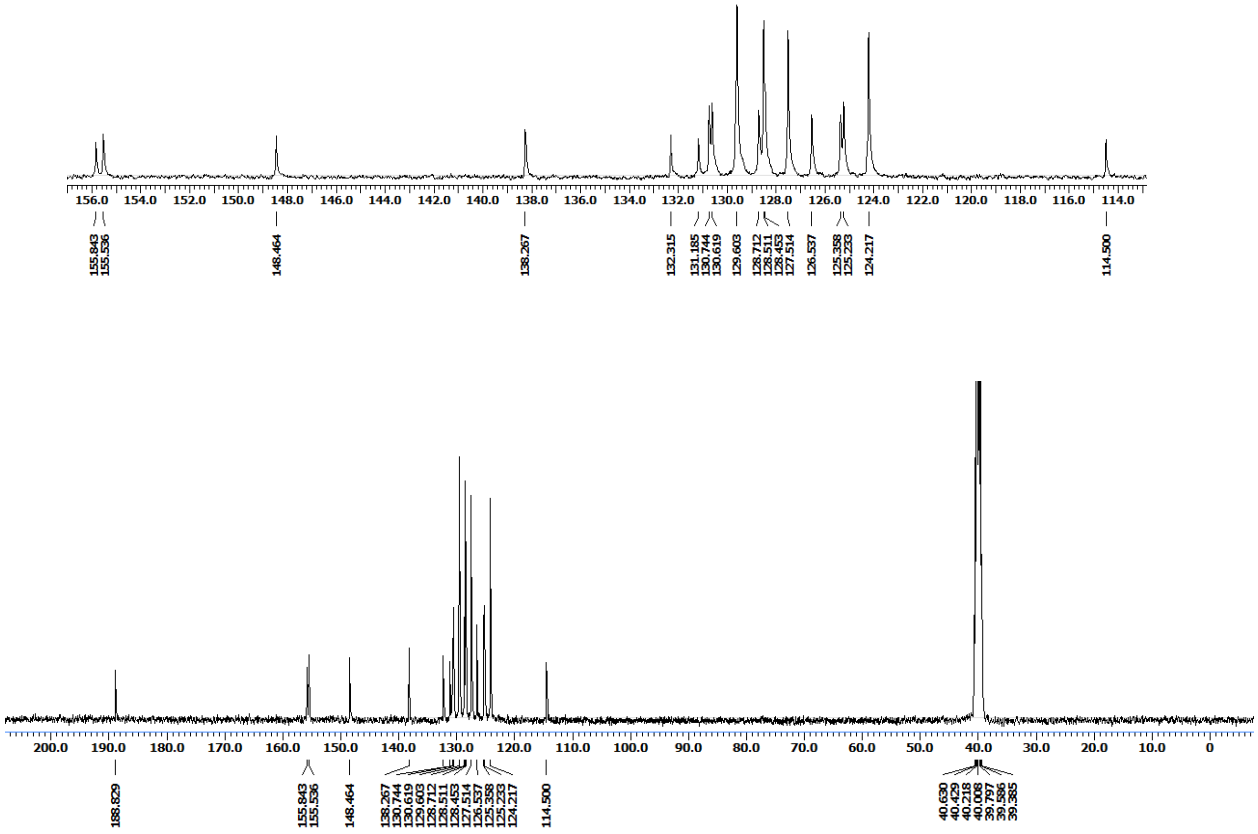

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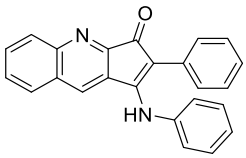

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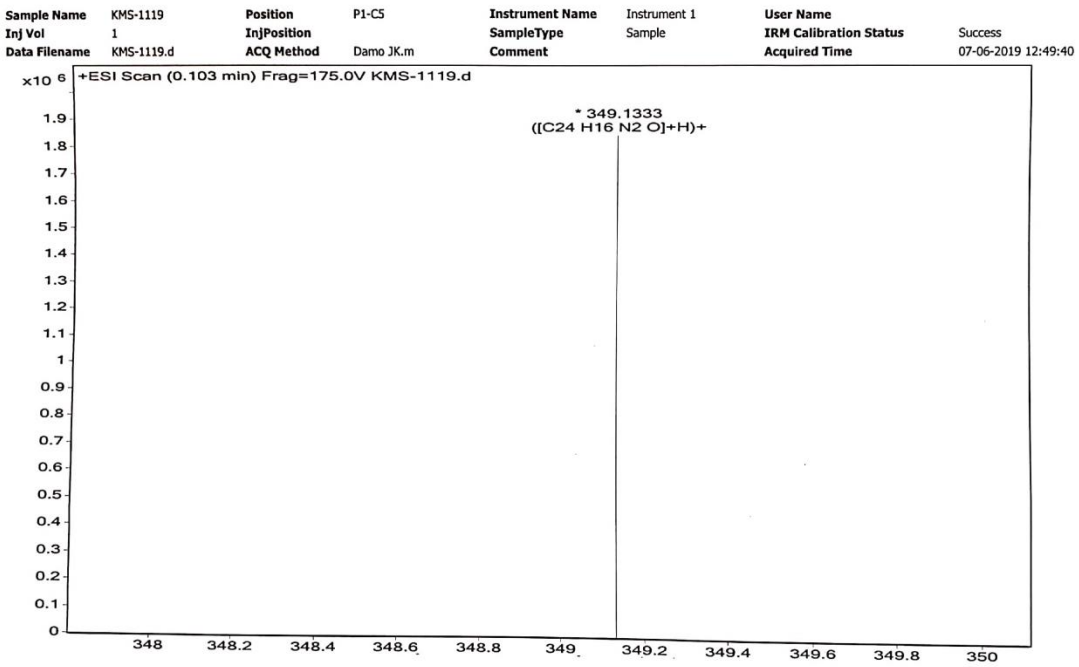

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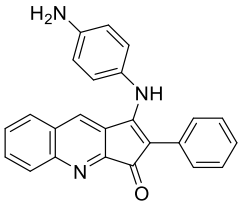

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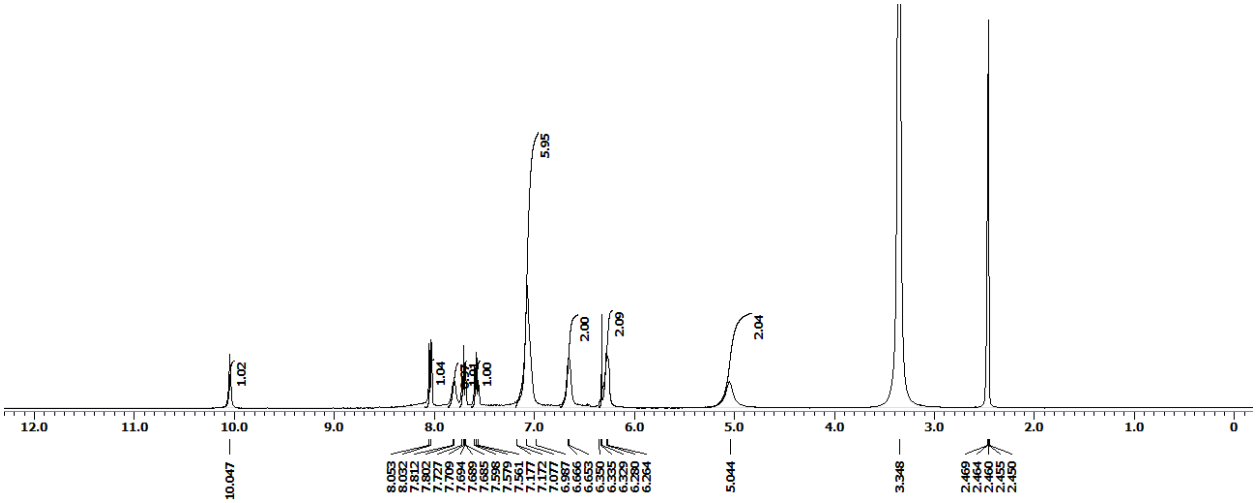

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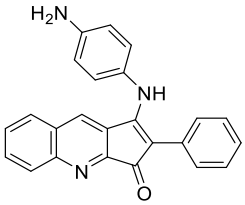

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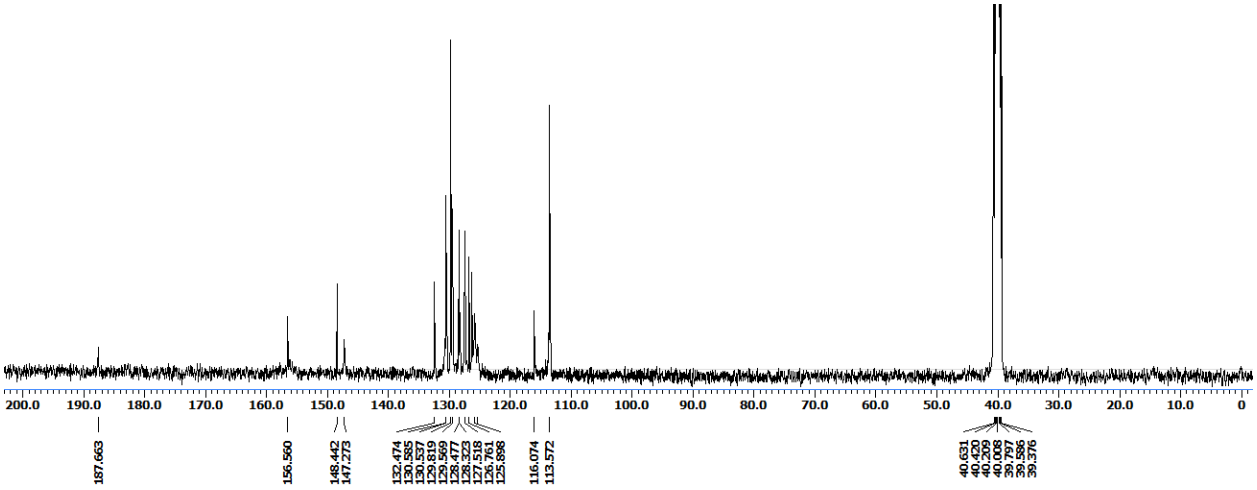

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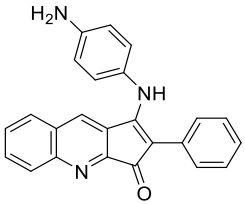

1-((4-Aminophenyl) amino)-2-phenyl-3*H*-cyclopenta[b]quinolin-3-one (3b)

Qualitative Compound Report

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Compound Table

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Compound Label	*m/z*	RT	Algorithm	Mass
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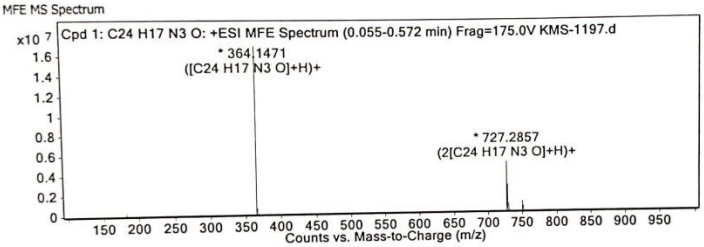
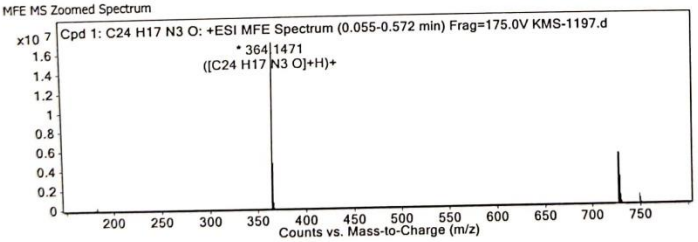


MFE MS Zoomed Spectrum



MS Spectrum Peak List

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365.1503	1	4592823.29	C24 H17 N3 O	(M+H)+
366.1537	1	619484.78	C24 H17 N3 O	(M+H)+
727.2857	1	5088761.5	C24 H17 N3 O	(2M+H)+
728.2891	1	2708773.73	C24 H17 N3 O	(2M+H)+
729.2925	1	750633.88	C24 H17 N3 O	(2M+H)+
730.2952	1	131284.13	C24 H17 N3 O	(2M+H)+
749.2682	1	919593.38	C24 H17 N3 O	(2M+Na)+
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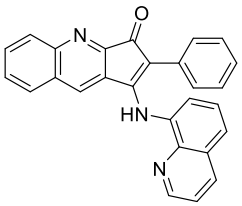
^{1}H NMR



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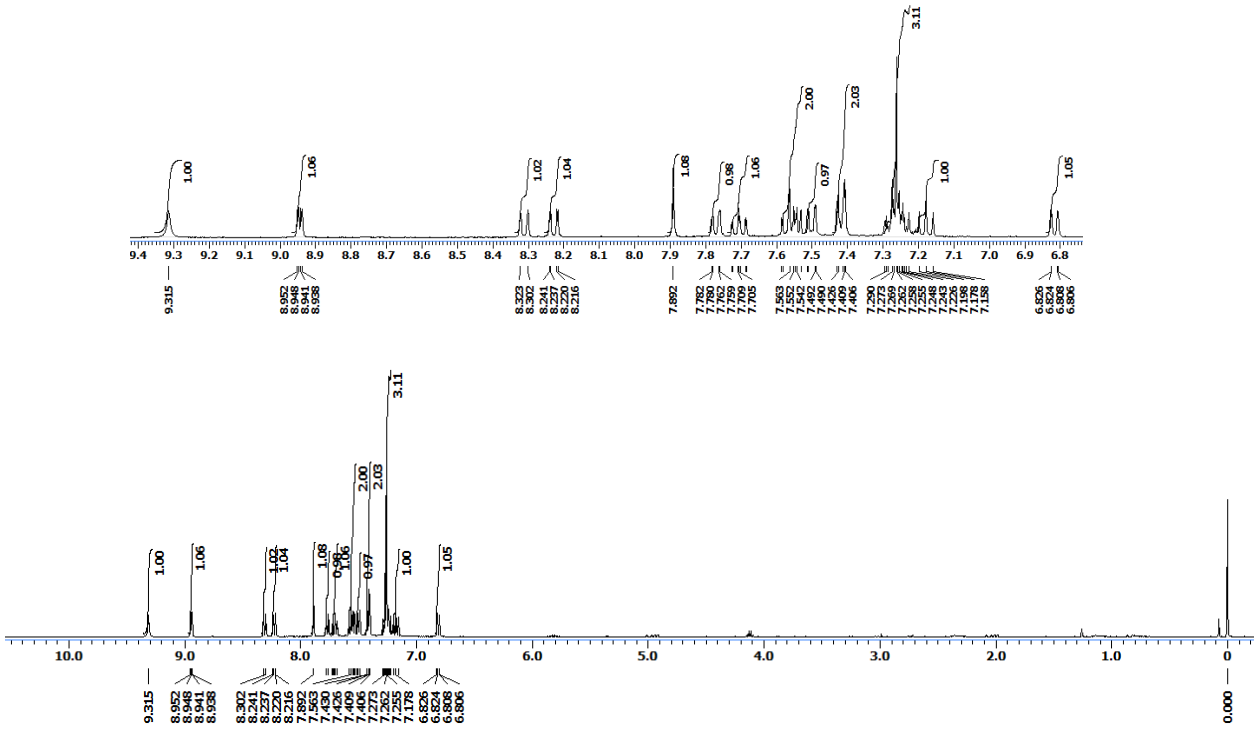
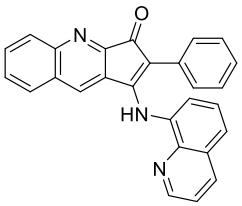


^{13}C NMR



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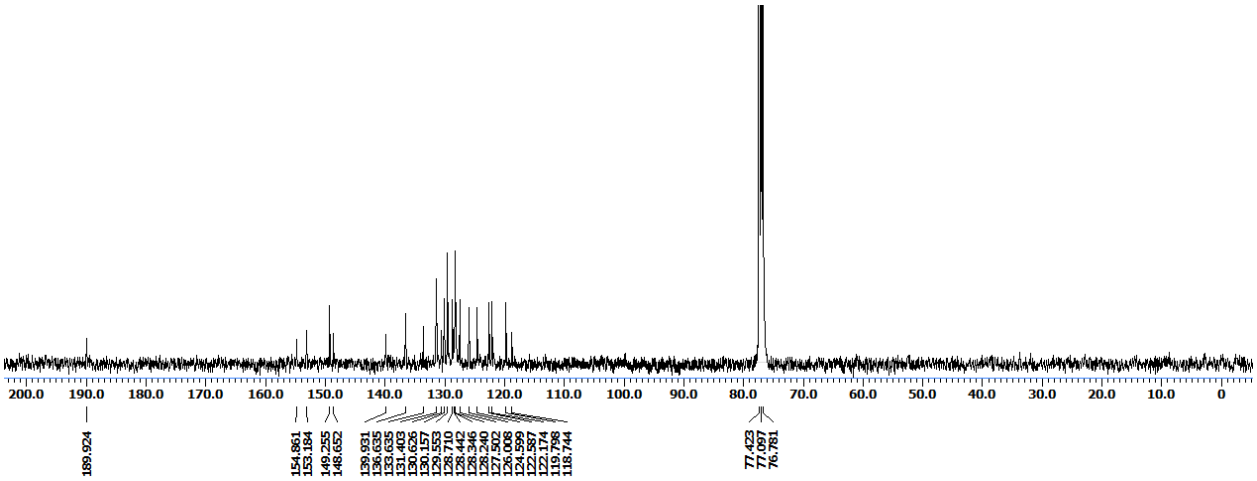

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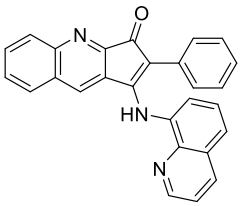

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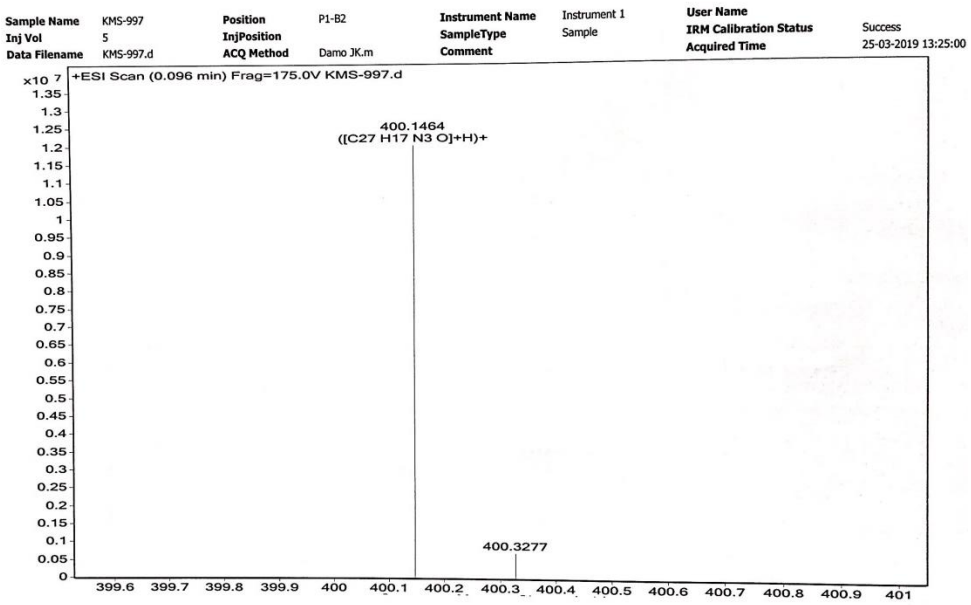
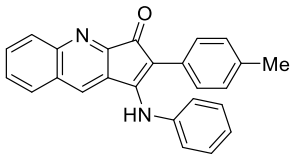


^{1}H NMR



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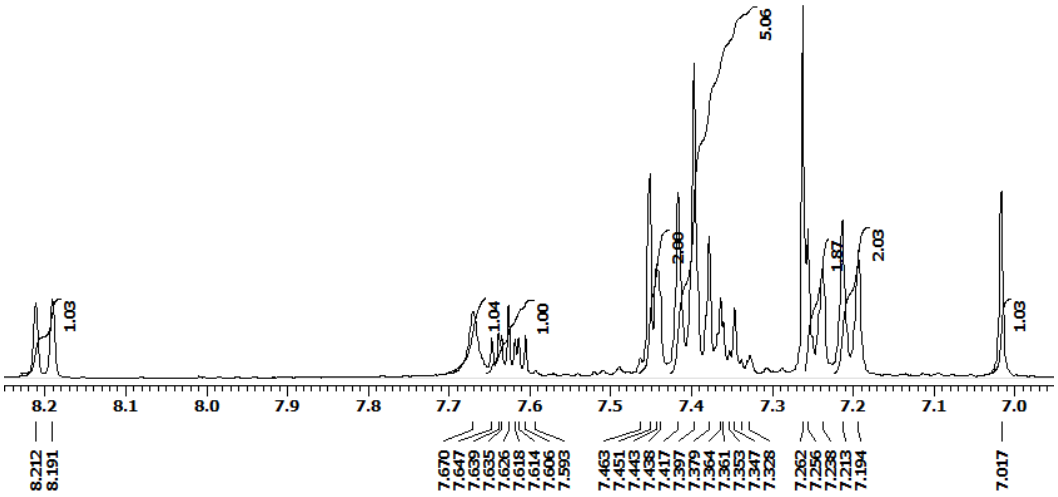

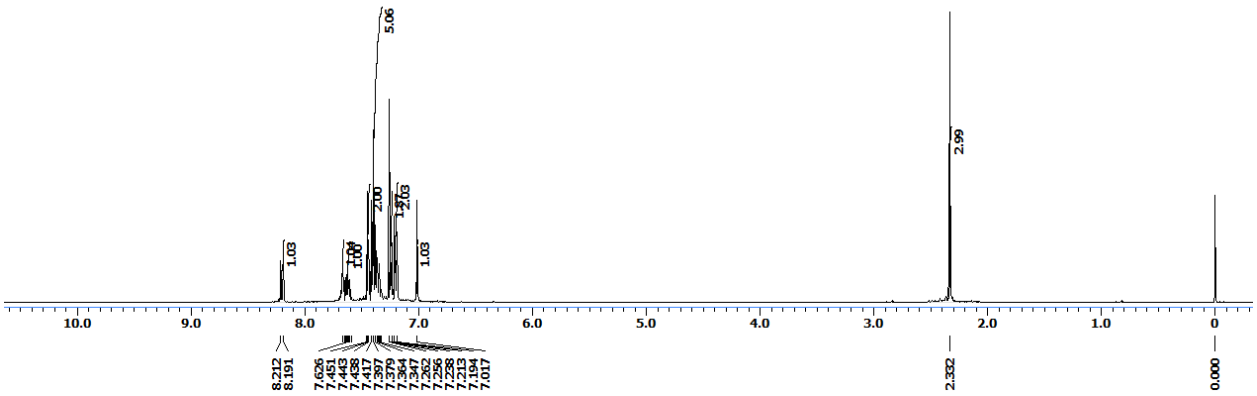

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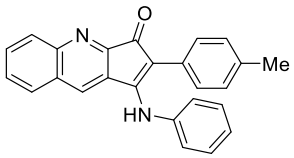

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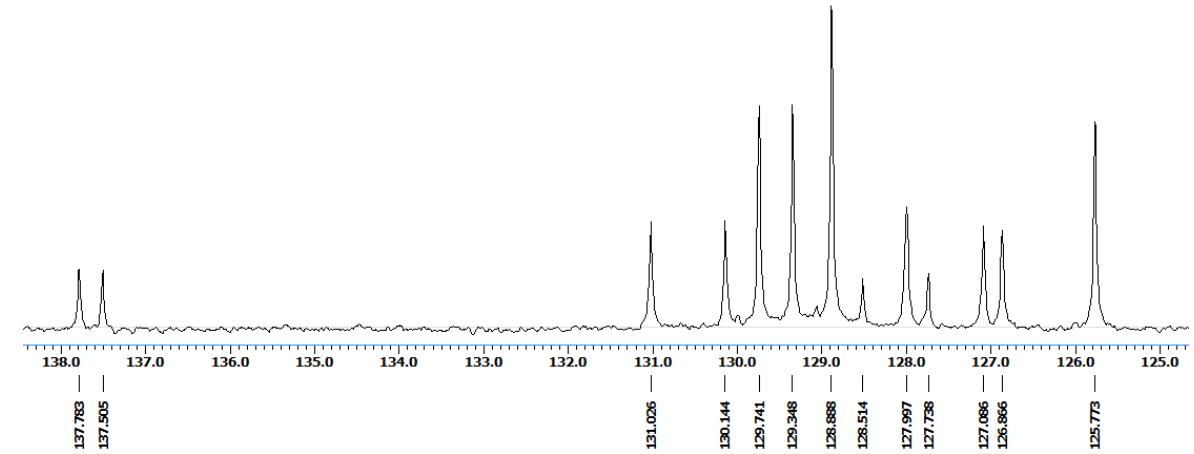

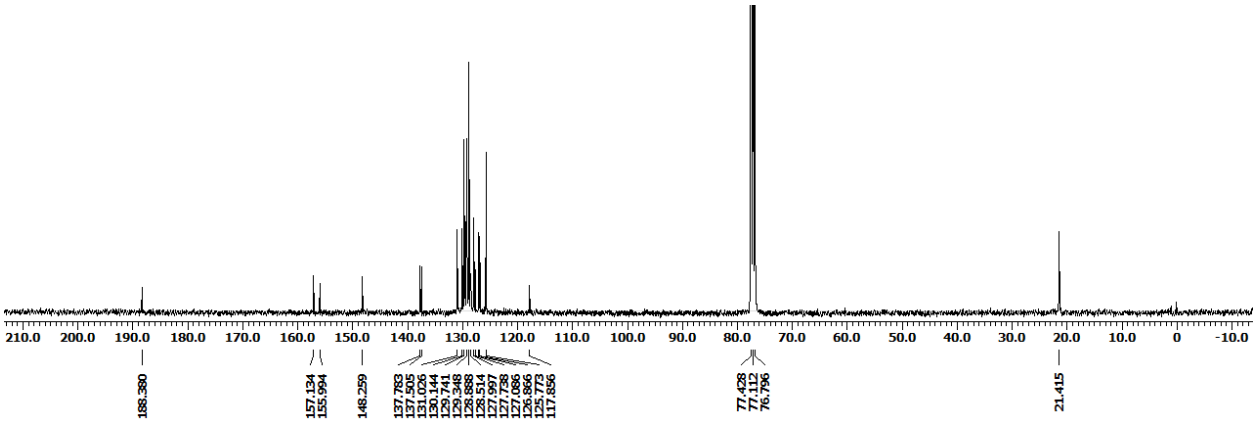

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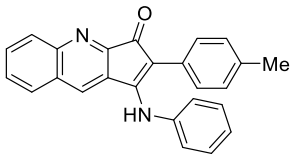

1-(Phenylamino)-2-(*p*-tolyl)-3*H*-cyclopenta[b]quinolin-3-one (3d)

Qualitative Compound Report

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Compound Table

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Compound Label	*m/z*	RT	Algorithm	Mass
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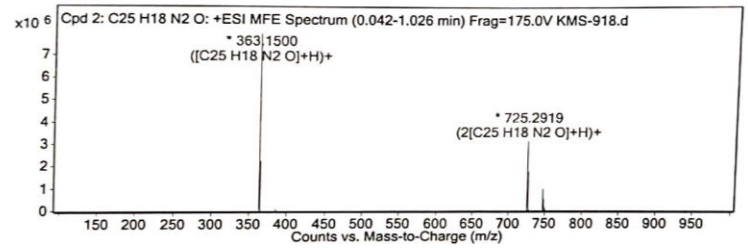
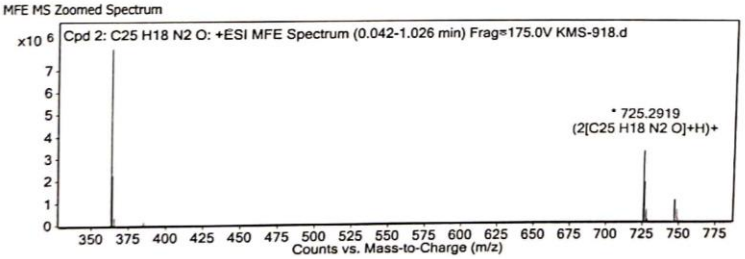
MFE MS Spectrum



MFE MS Zoomed Spectrum



MS Spectrum Peak List

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365.1573	1	328692.46	C25 H18 N2 O	(M+H)+
385.1314	1	134931.13	C25 H18 N2 O	(M+Na)+
725.2919	1	3170710	C25 H18 N2 O	(2M+H)+
726.2951	1	1795642.7	C25 H18 N2 O	(2M+H)+
727.2983	1	514764.84	C25 H18 N2 O	(2M+H)+
747.2738	1	986285.94	C25 H18 N2 O	(2M+Na)+
748.2768	1	538194.11	C25 H18 N2 O	(2M+Na)+
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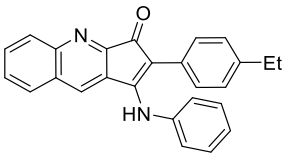
^{1}H NMR



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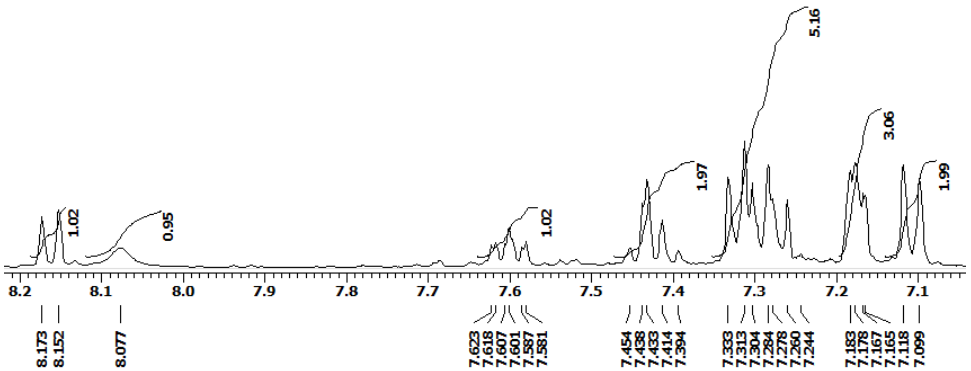
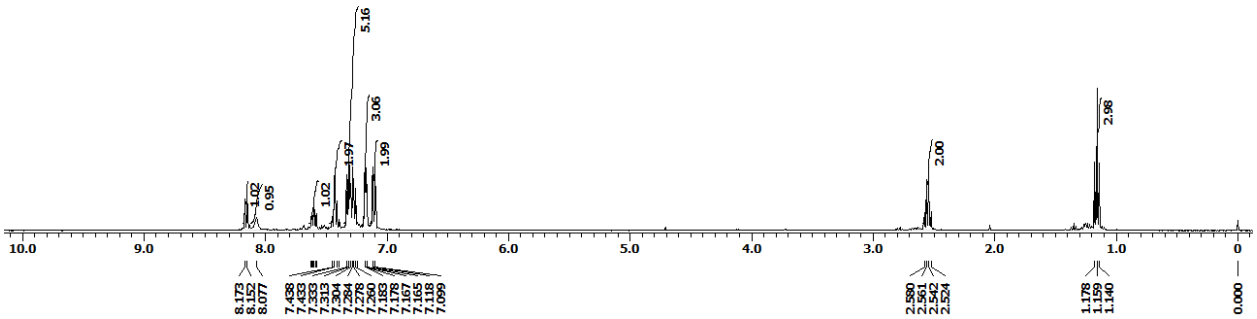
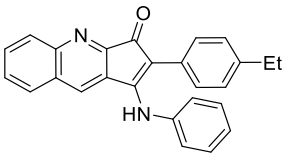
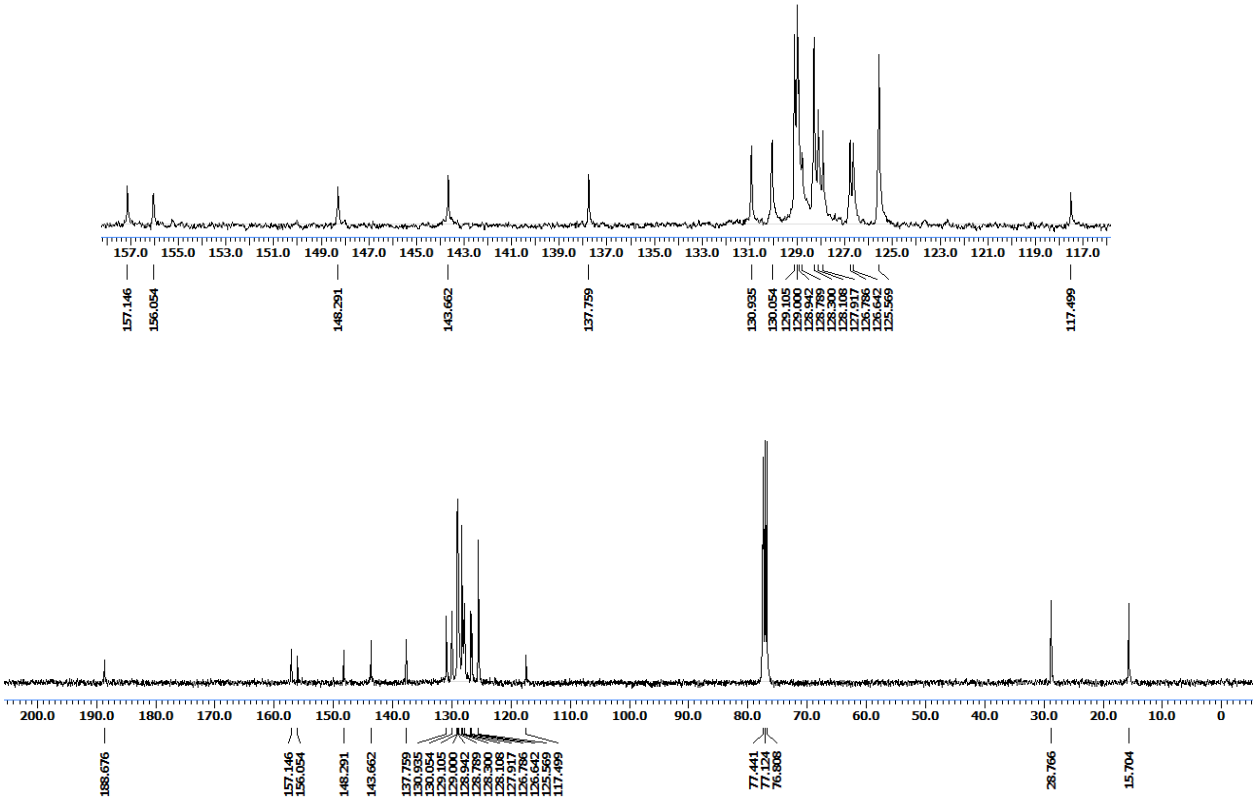




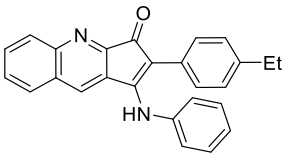
^{13}C NMR



2-(4-Ethylphenyl)-1-(phenylamino)-3*H*-cyclopenta[b]quinolin-3-one (3e)



HRMS



2-(4-Ethylphenyl)-1-(phenylamino)-3*H*-cyclopenta[b]quinolin-3-one (3e)

Qualitative Compound Report

Data File	KMS-1110.d	**Sample Name**	KMS-1110
Sample Type	Sample	**Position**	P1-A1
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	29-05-2019 12:49:56
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

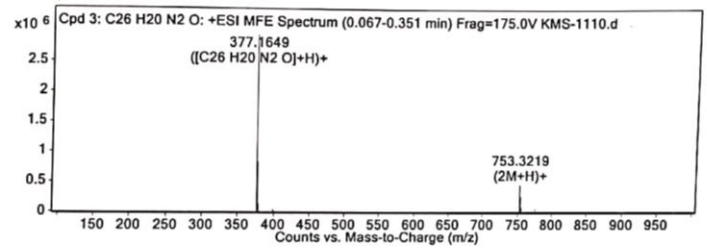
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

Compound Table

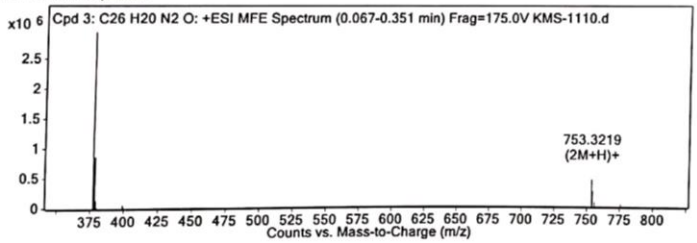
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 3: C26 H20 N2 O	0.101	376.1577	C26 H20 N2 O	C26 H20 N2 O	-0.32	C26 H20 N2 O

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 3: C26 H20 N2 O	377.1649	0.101	Find by Molecular Feature	376.1577

MFE MS Spectrum



MFE MS Zoomed Spectrum

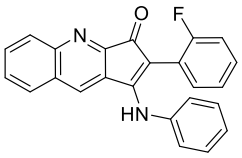


MS Spectrum Peak List

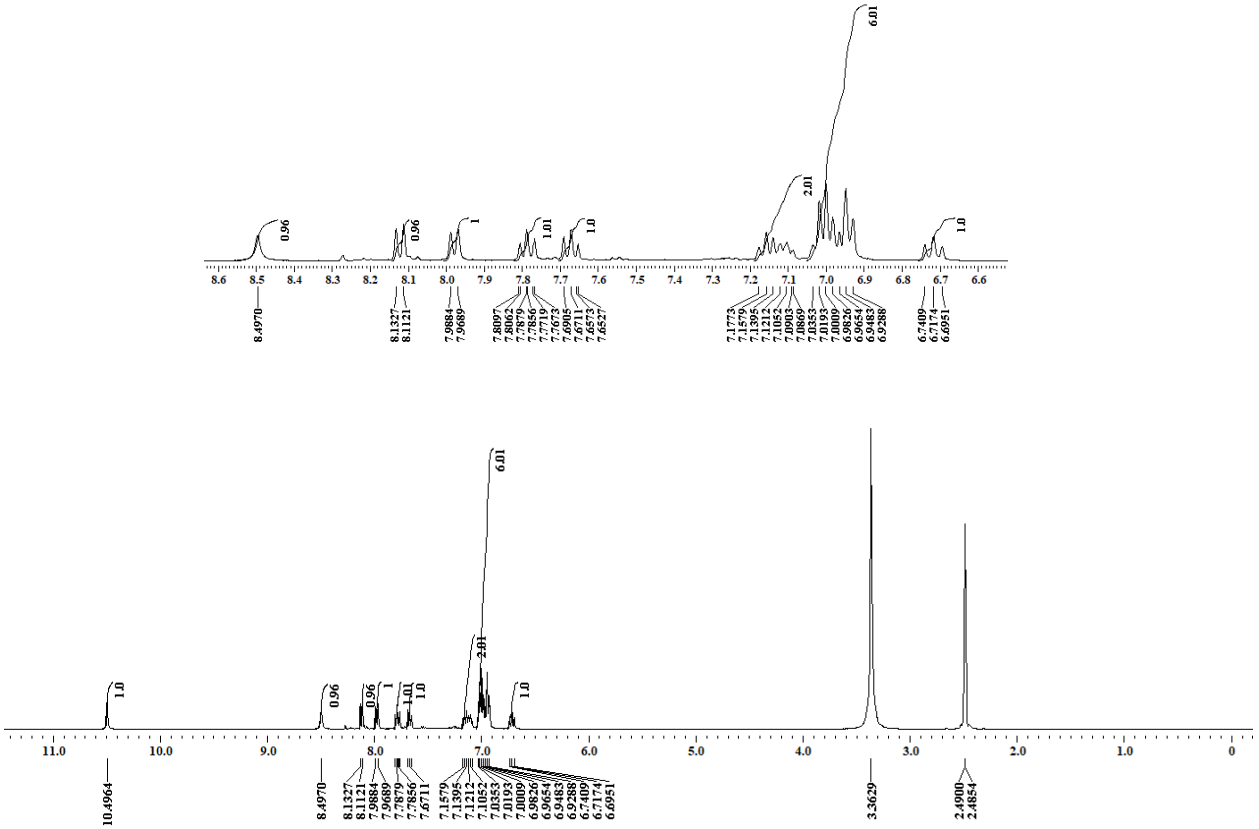
m/z	z	Abund	Formula	Ion
377.1649	1	2933440.5	C26 H20 N2 O	(M+H)+
378.1683	1	838827.12	C26 H20 N2 O	(M+H)+
379.1716	1	131652.02	C26 H20 N2 O	(M+H)+
380.1754	1	14475	C26 H20 N2 O	(M+H)+
399.1478	1	44068.19	C26 H20 N2 O	(M+Na)+
753.3219	1	456147.94		(2M+H)+
754.3249	1	254732.24		(2M+H)+
755.3273	1	71086.96		(2M+H)+
775.3032	1	38569.2		(2M+Na)+
776.3064	1	22415.47		(2M+Na)+

--- End Of Report ---

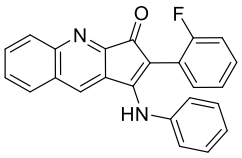
^{1}H NMR



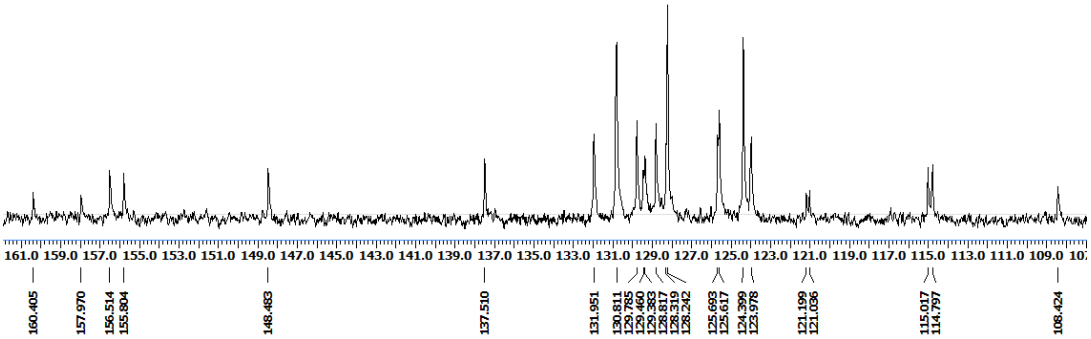
2-(2-Fluorophenyl)-1-(phenylamino)-3*H*-cyclopenta[b]quinolin-3-one (3f)

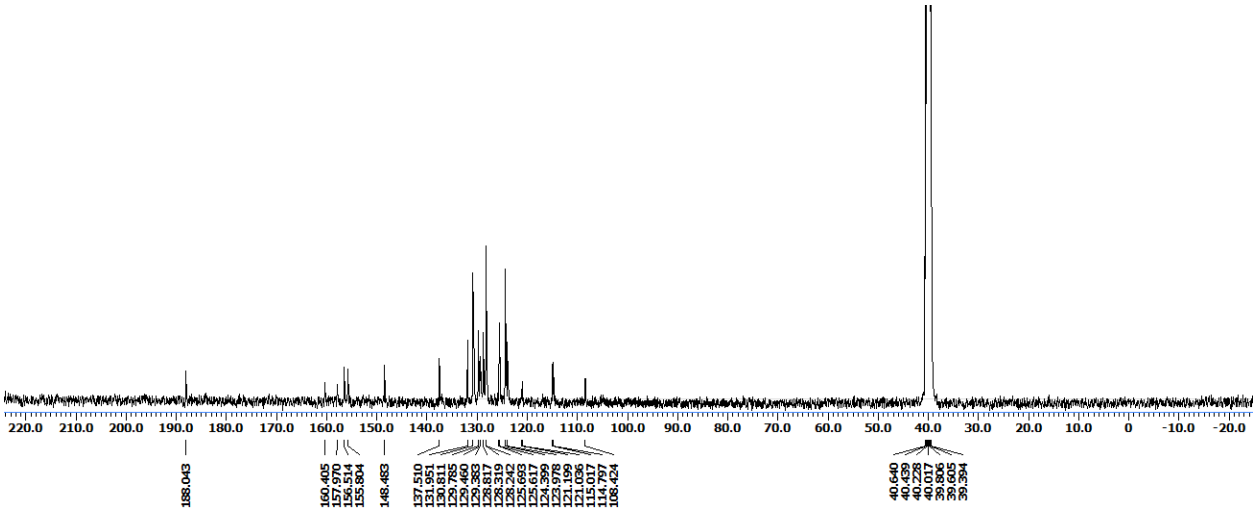


^{13}C NMR

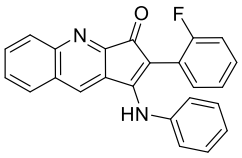


2-(2-Fluorophenyl)-1-(phenylamino)-3*H*-cyclopenta[b]quinolin-3-one (3f)

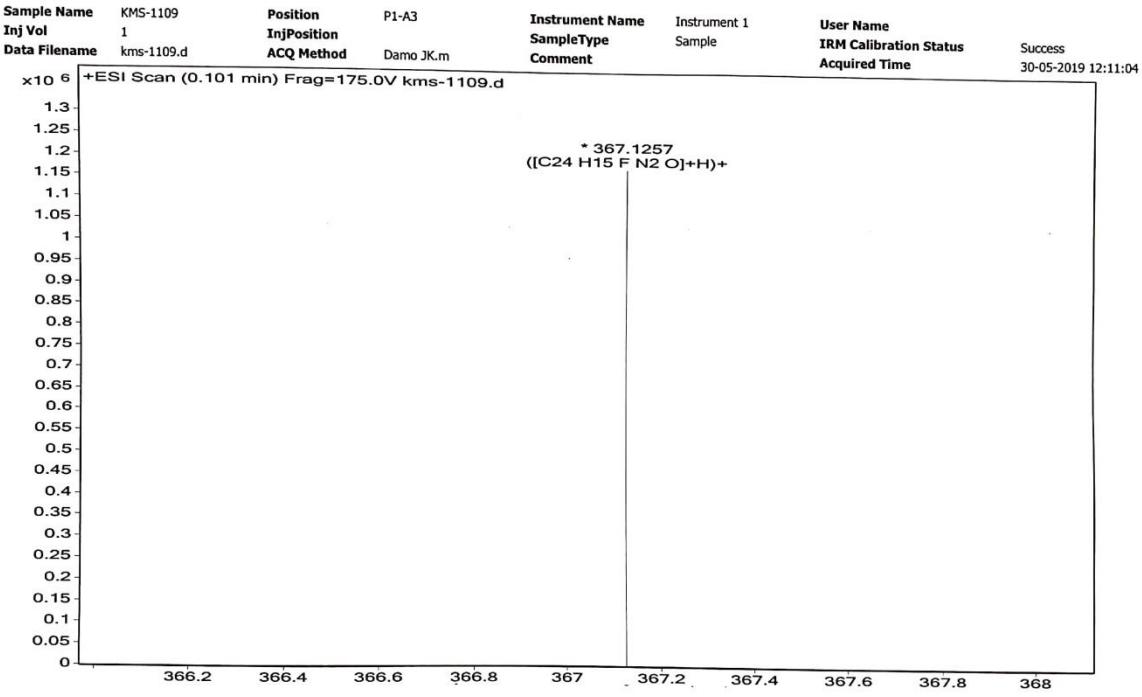




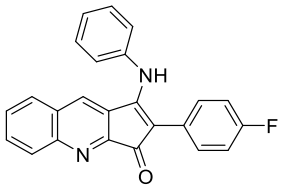
HRMS



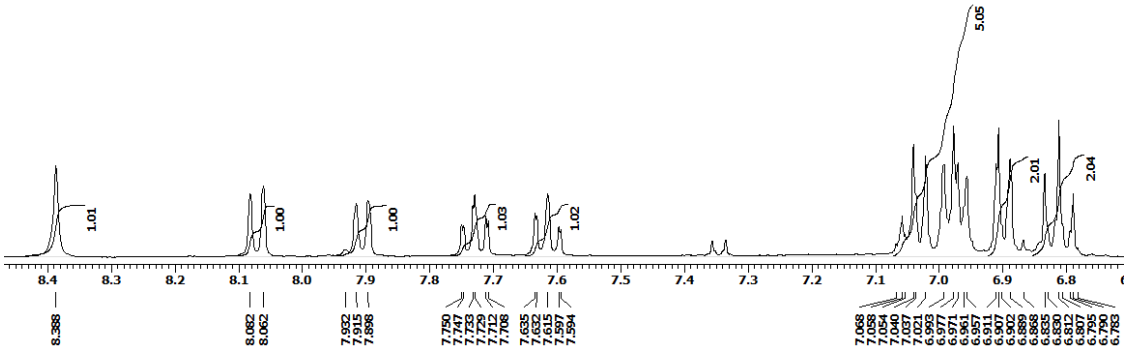
2-(2-Fluorophenyl)-1-(phenylamino)-3*H*-cyclopenta[b]quinolin-3-one (3f)

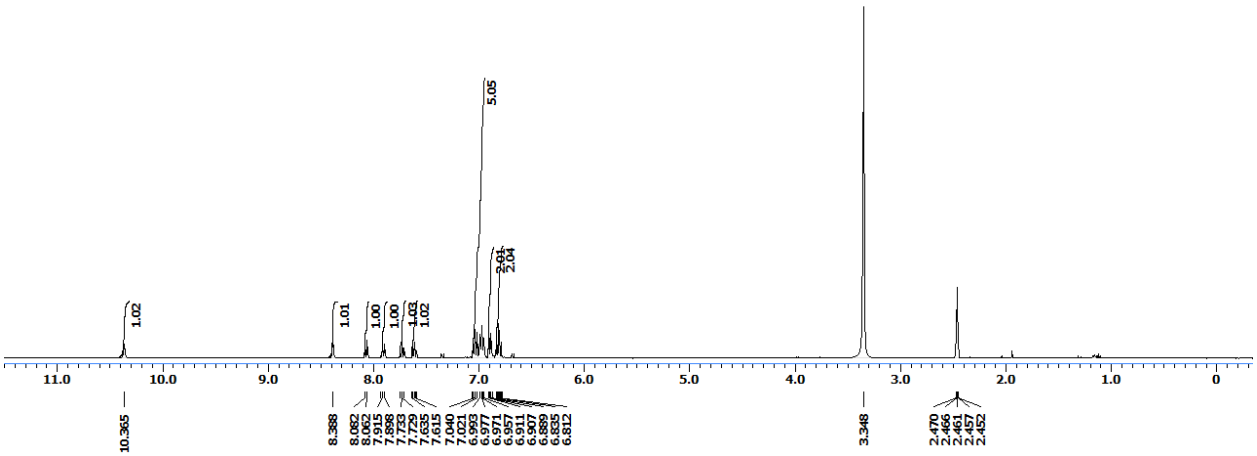


^{1}H NMR

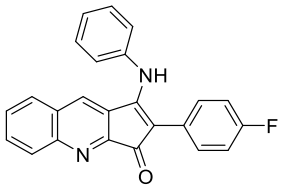


2-(4-Fluorophenyl)-1-(phenylamino)-3*H*-cyclopenta[b]quinolin-3-one (3g)

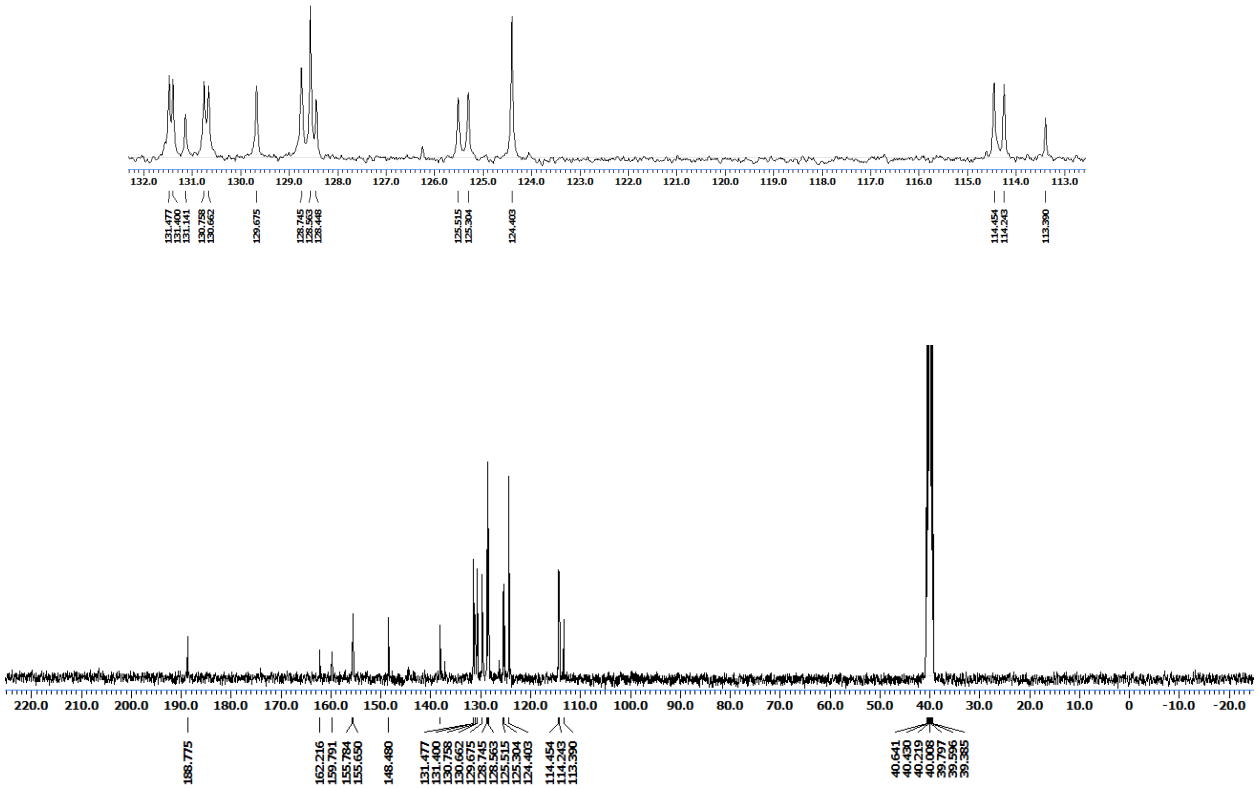




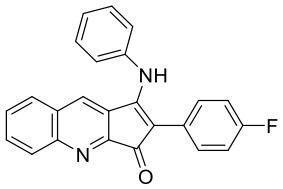
^{13}C NMR



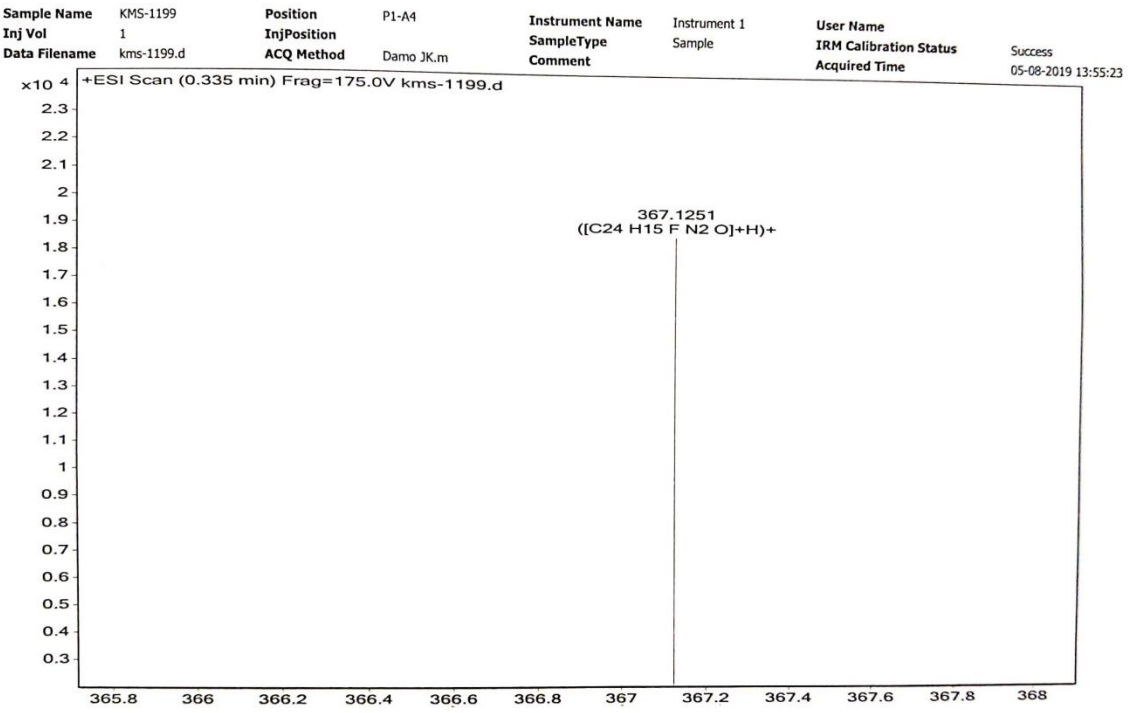
2-(4-Fluorophenyl)-1-(phenylamino)-3*H*-cyclopenta[b]quinolin-3-one (3g)



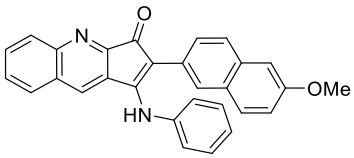
HRMS



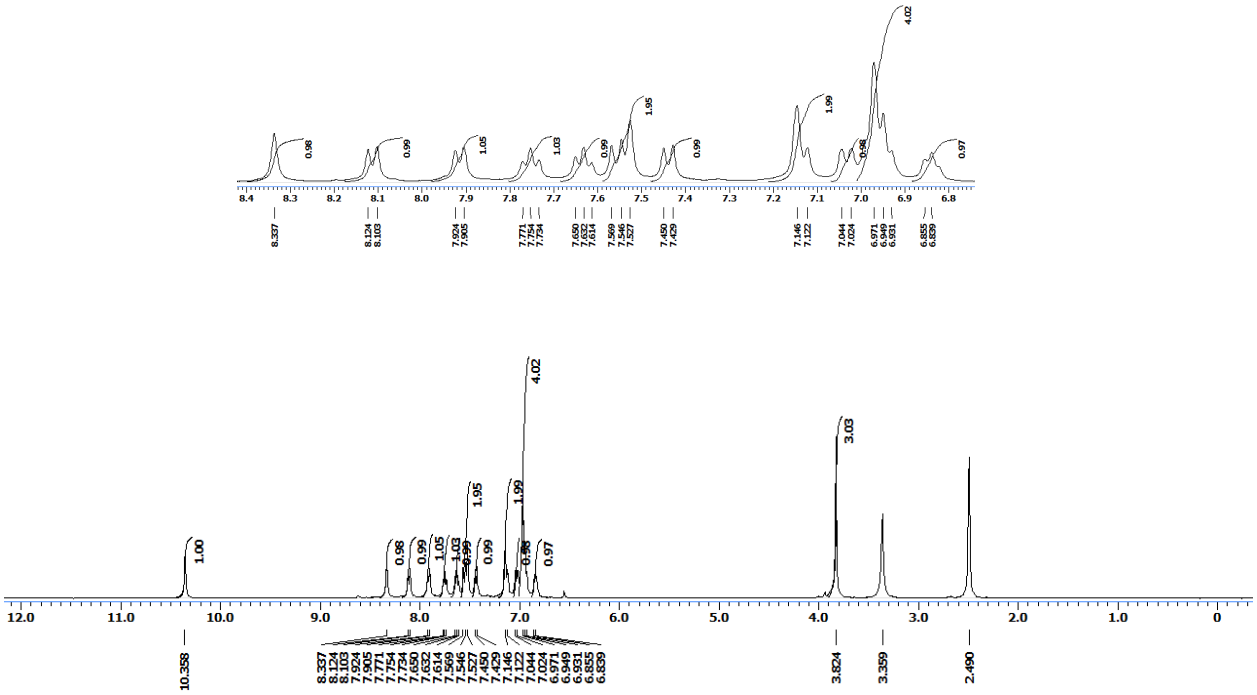
2-(4-Fluorophenyl)-1-(phenylamino)-3*H*-cyclopenta[b]quinolin-3-one (3g)



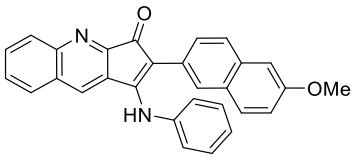
^{1}H NMR



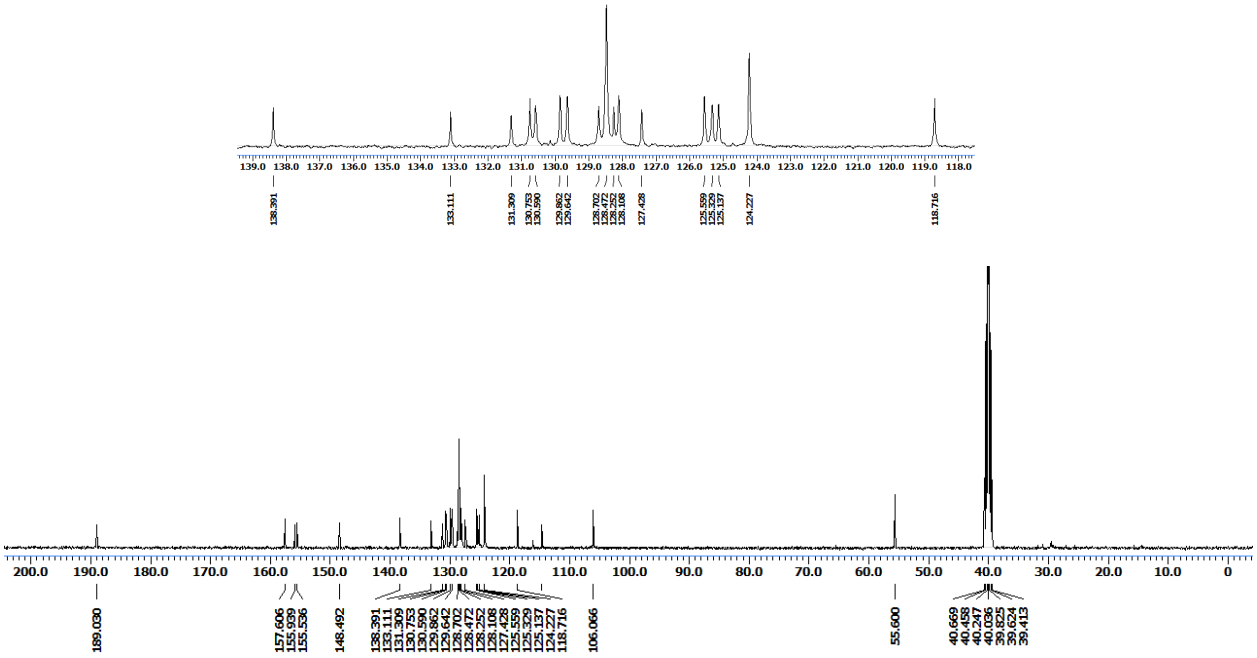
2-(6-Methoxynaphthalen-2-yl)-1-(phenylamino)-3*H*-cyclopenta[b]quinolin-3-one (3h)



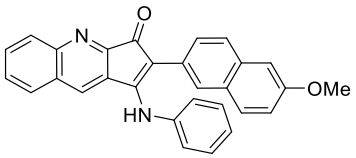
^{13}C NMR



2-(6-Methoxynaphthalen-2-yl)-1-(phenylamino)-3*H*-cyclopenta[b]quinolin-3-one (3h)



HRMS



2-(6-Methoxynaphthalen-2-yl)-1-(phenylamino)-3*H*-cyclopenta[b]quinolin-3-one (3h)

Qualitative Compound Report

Data File	KMS-1113.d	**Sample Name**	KMS-1113
Sample Type	Sample	**Position**	P1-A1
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	30-05-2019 12:07:08
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

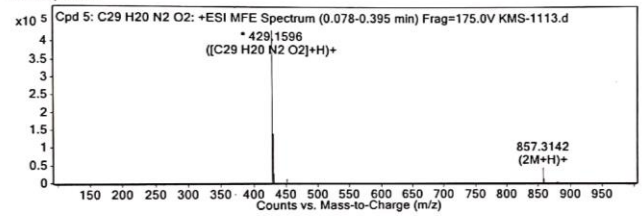
Sample Group **Info.**
Acquisition SW 6200 series TOF/6500 series
Version Q-TOF B.05.01 (B5125.1)

Compound Table

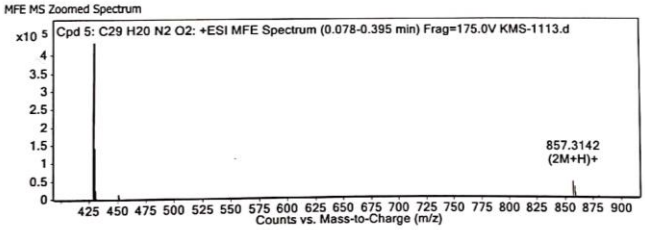
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 5: C29 H20 N2 O2	0.101	428.1524	C29 H20 N2 O2	C29 H20 N2 O2	0.2	C29 H20 N2 O2

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 5: C29 H20 N2 O2	429.1596	0.101	Find by Molecular Feature	428.1524

MFE MS Spectrum



MFE MS Zoomed Spectrum

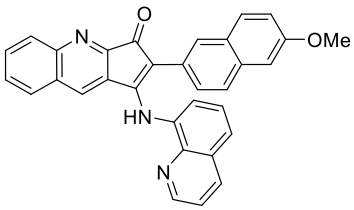


MS Spectrum Peak List

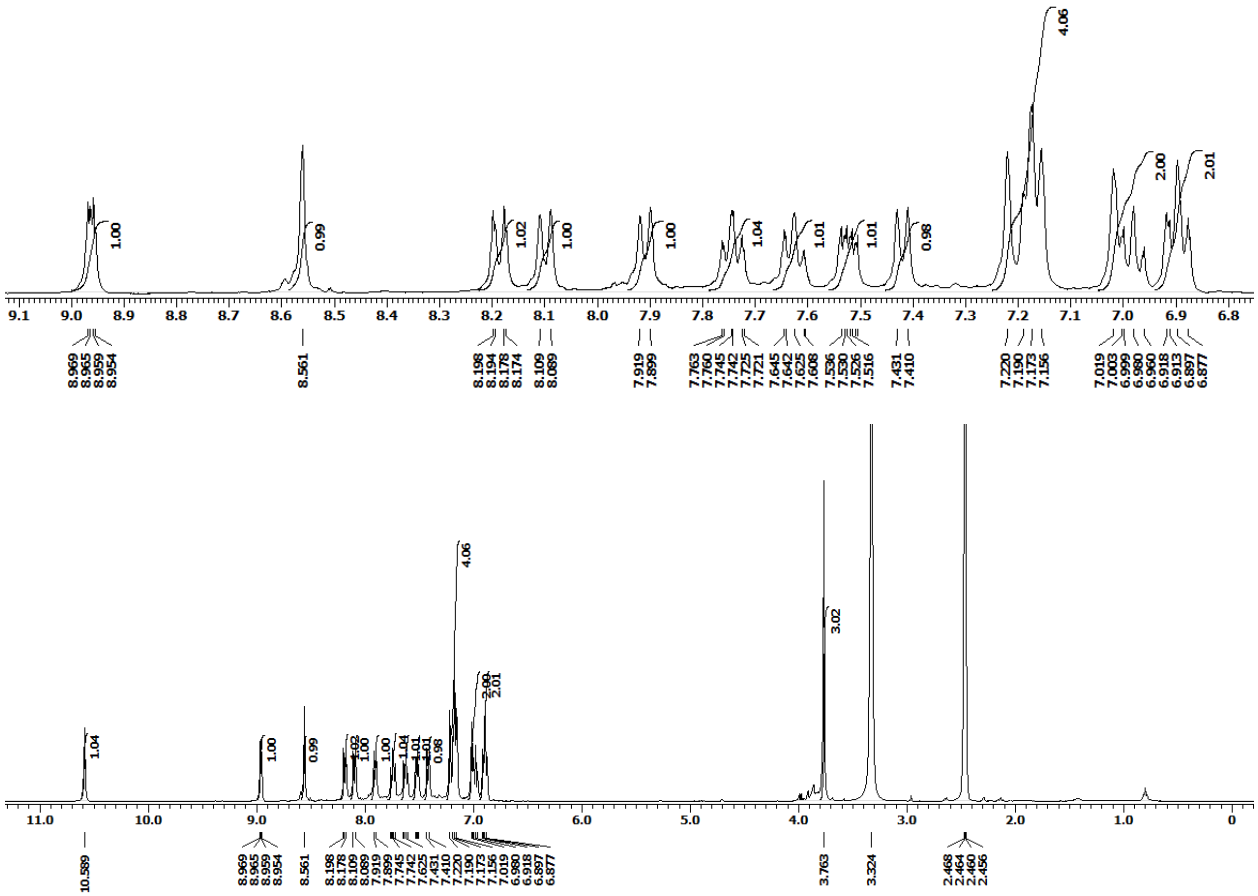
m/z	z	Abund	Formula	Ion
429.1596	1	434644.41	C29 H20 N2 O2	(M+H)+
430.1634	1	140628.49	C29 H20 N2 O2	(M+H)+
431.1651	1	25943.31	C29 H20 N2 O2	(M+H)+
432.1672	1	3035.27	C29 H20 N2 O2	(M+H)+
451.1417	1	11851.14	C29 H20 N2 O2	(M+Na)+
452.1456	1	3885.93	C29 H20 N2 O2	(M+Na)+
857.3142	1	42406.5		(2M+H)+
858.3159	1	28836.88		(2M+H)+
859.3178	1	10928.33		(2M+H)+
879.2929	1	3062.48		(2M+Na)+

--- End Of Report ---

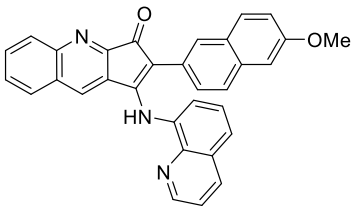
^{1}H NMR



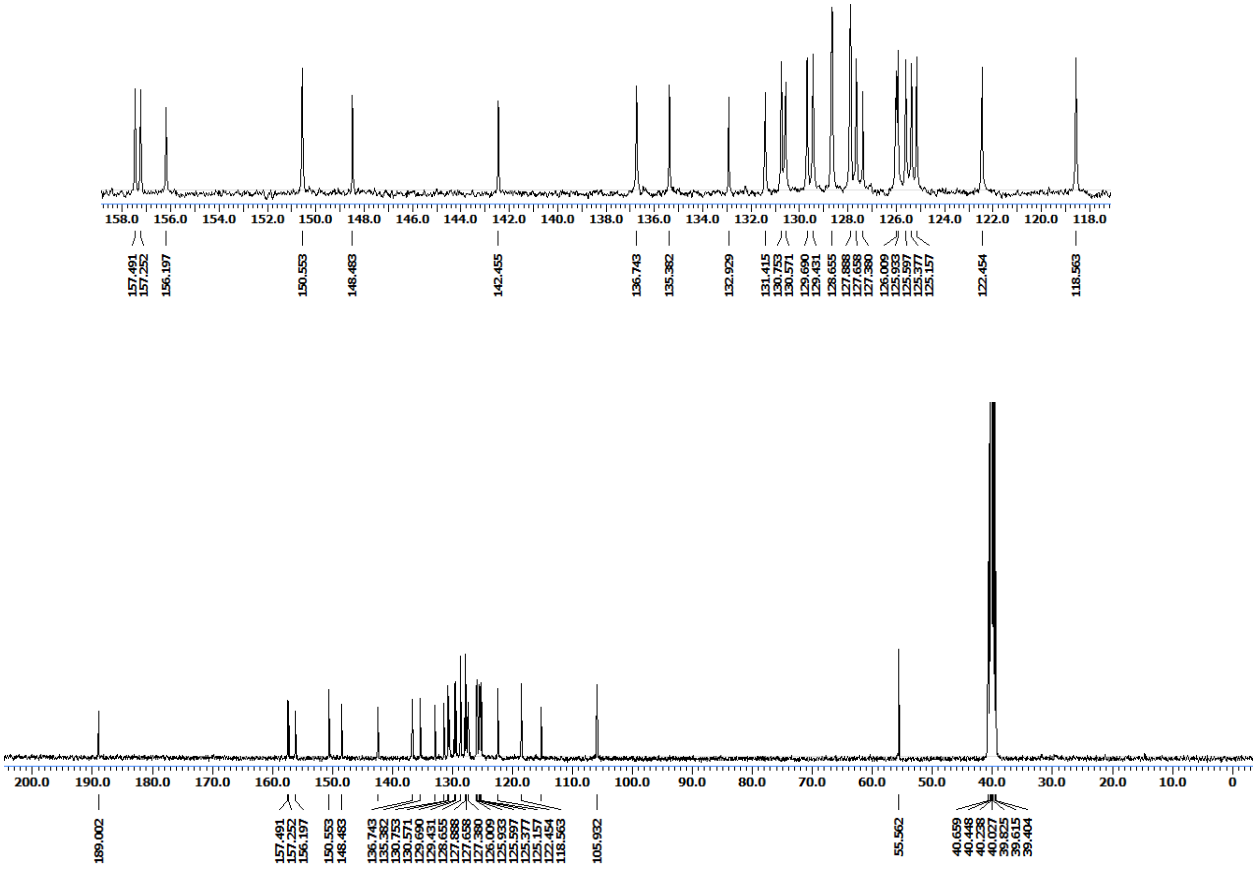
2-(6-Methoxynaphthalen-2-yl)-1-(quinolin-8-ylamino)-3*H*-cyclopenta[b]quinolin-3-one (3i)



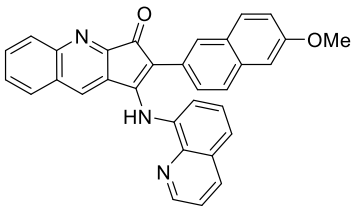
^{13}C NMR



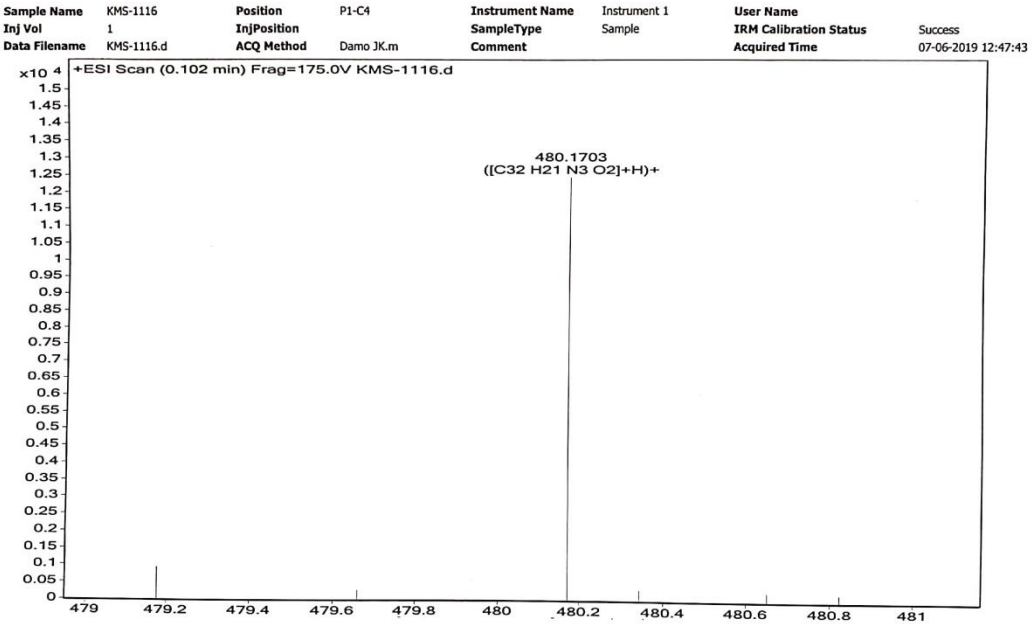
2-(6-Methoxynaphthalen-2-yl)-1-(quinolin-8-ylamino)-3*H*-cyclopenta[b]quinolin-3-one (3i)



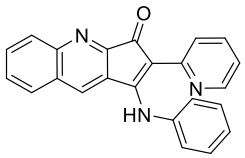
HRMS



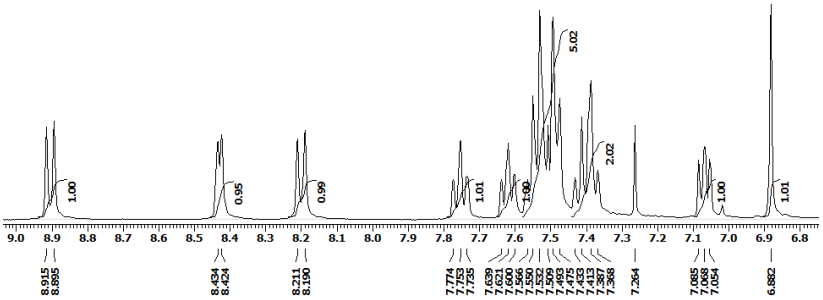
2-(6-Methoxynaphthalen-2-yl)-1-(quinolin-8-ylamino)-3*H*-cyclopenta[b]quinolin-3-one (3i)

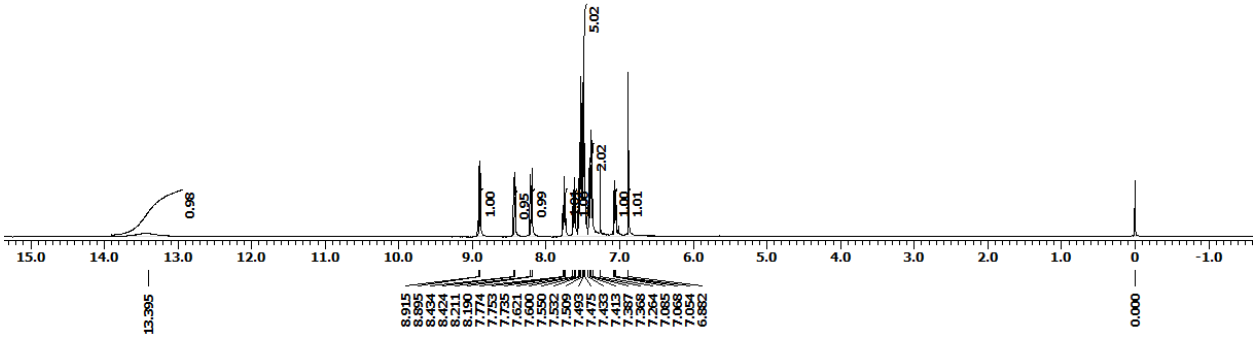


^{1}H NMR

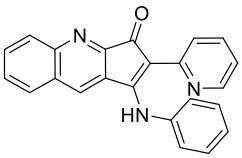


1-(Phenylamino)-2-(pyridin-2-yl)-3*H*-cyclopenta[b]quinolin-3-one (3j)

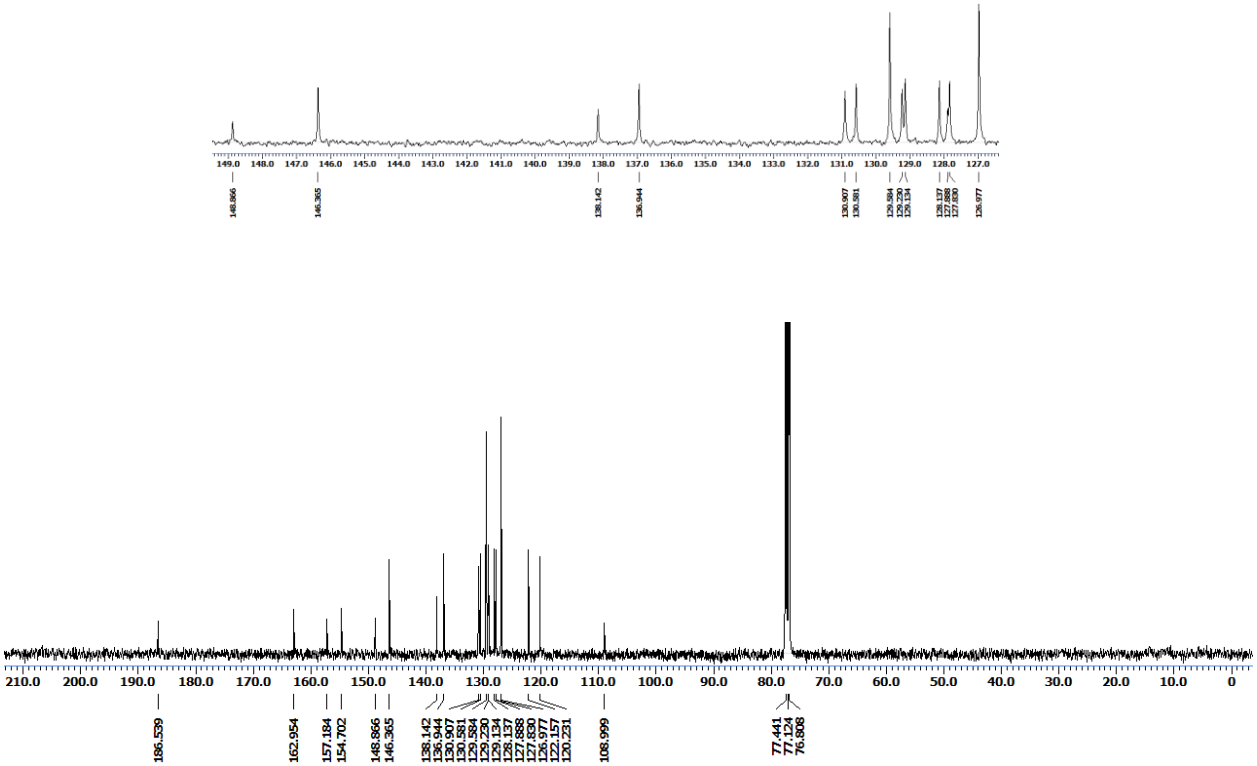




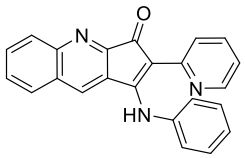
^{13}C NMR



1-(Phenylamino)-2-(pyridin-2-yl)-3*H*-cyclopenta[b]quinolin-3-one (3j)



HRMS



1-(Phenylamino)-2-(pyridin-2-yl)-3*H*-cyclopenta[b]quinolin-3-one (3j)

Qualitative Compound Report

Data File	KMS-1112.d	**Sample Name**	KMS-1112
Sample Type	Sample	**Position**	P1-A4
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	30-05-2019 12:13:01
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

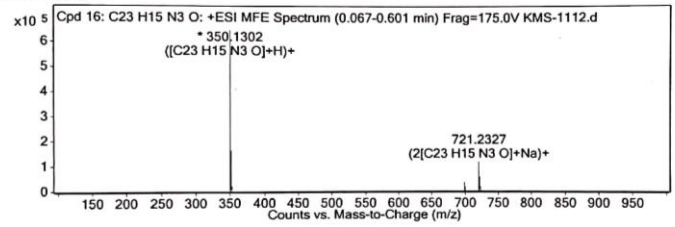
Sample Group **Info.**
Acquisition SW 6200 series TOF/6500 series
Version Q-TOF B.05.01 (B5125.1)

Compound Table

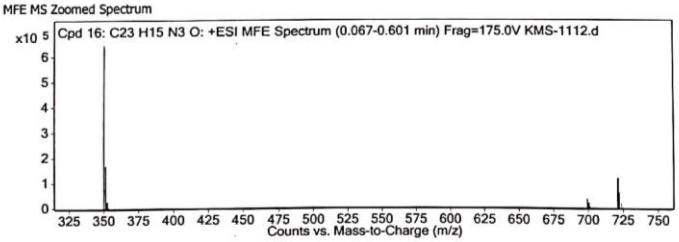
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 16: C23 H15 N3 O	0.187	349.122	C23 H15 N3 O	C23 H15 N3 O	-1.31	C23 H15 N3 O

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 16: C23 H15 N3 O	350.1302	0.187	Find by Molecular Feature	349.122

MFE MS Spectrum



MFE MS Zoomed Spectrum

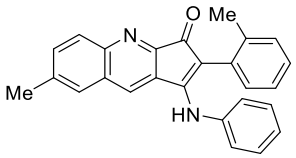


MS Spectrum Peak List

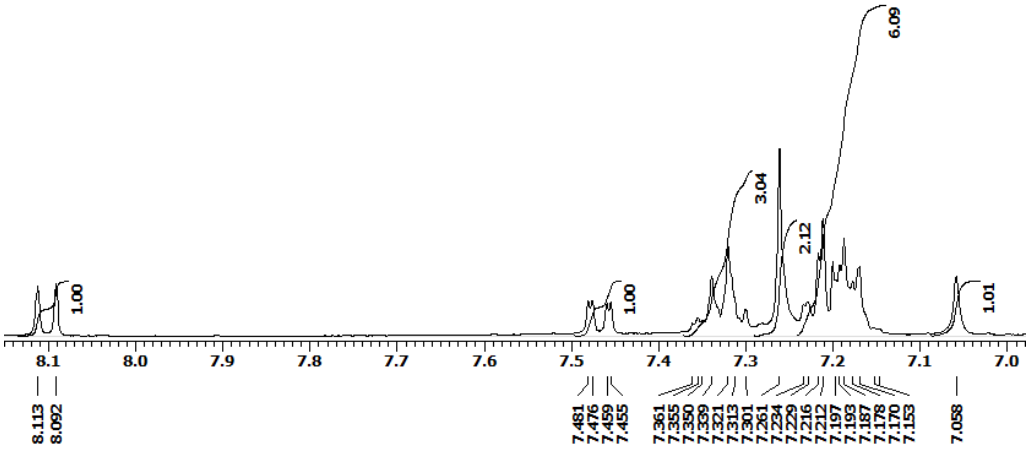
m/z	z	Abund	Formula	Ion
350.1302	1	646199.63	C23 H15 N3 O	(M+H)+
351.1298	1	164795.89	C23 H15 N3 O	(M+H)+
352.1358	1	20909.77	C23 H15 N3 O	(M+H)+
699.2501	1	33132.85	C23 H15 N3 O	(2M+H)+
700.2543	1	17838.83	C23 H15 N3 O	(2M+H)+
701.2595	1	4427.6	C23 H15 N3 O	(2M+H)+
721.2327	1	116313.23	C23 H15 N3 O	(2M+Na)+
722.238	1	55610.4	C23 H15 N3 O	(2M+Na)+
723.2402	1	16069.32	C23 H15 N3 O	(2M+Na)+
724.2424	1	2598.13	C23 H15 N3 O	(2M+Na)+

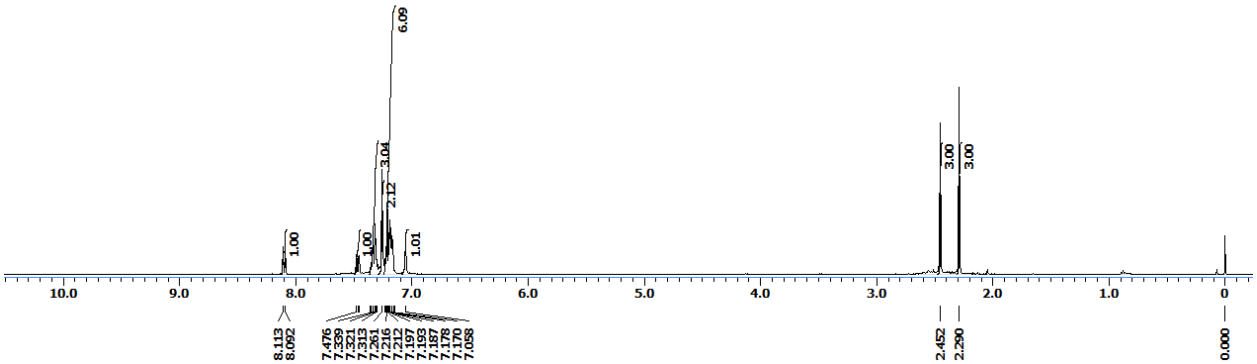
--- End Of Report ---

^{1}H NMR

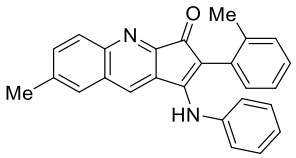


7-Methyl-1-(phenylamino)-2-(*o*-tolyl)-3*H*-cyclopenta[b]quinolin-3-one (3k)

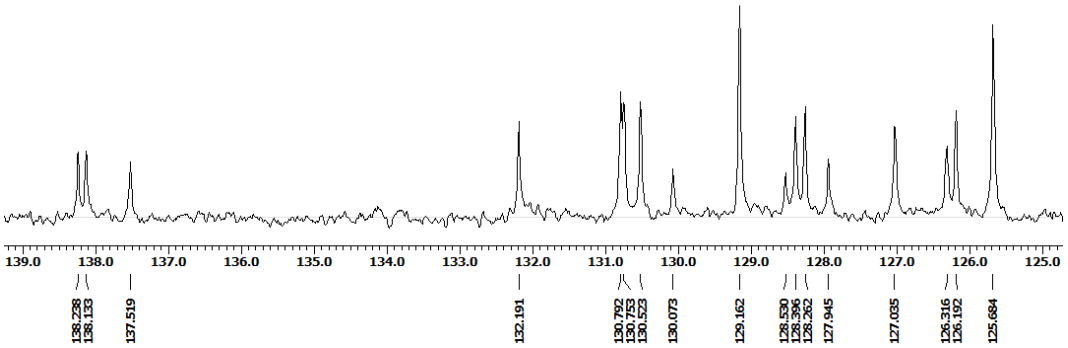


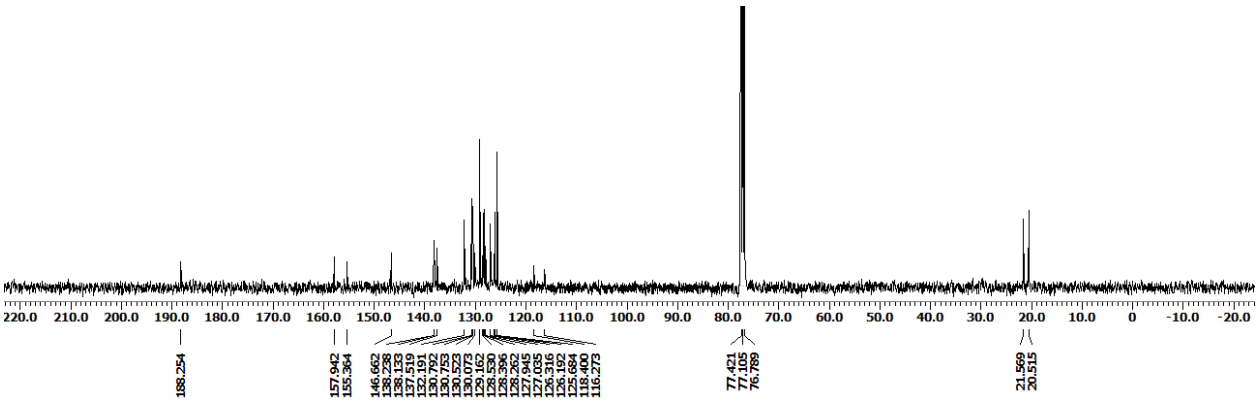


^{13}C NMR

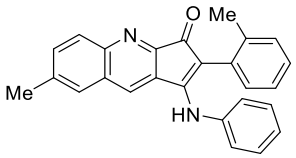


7-Methyl-1-(phenylamino)-2-(*o*-tolyl)-3*H*-cyclopenta[b]quinolin-3-one (3k)

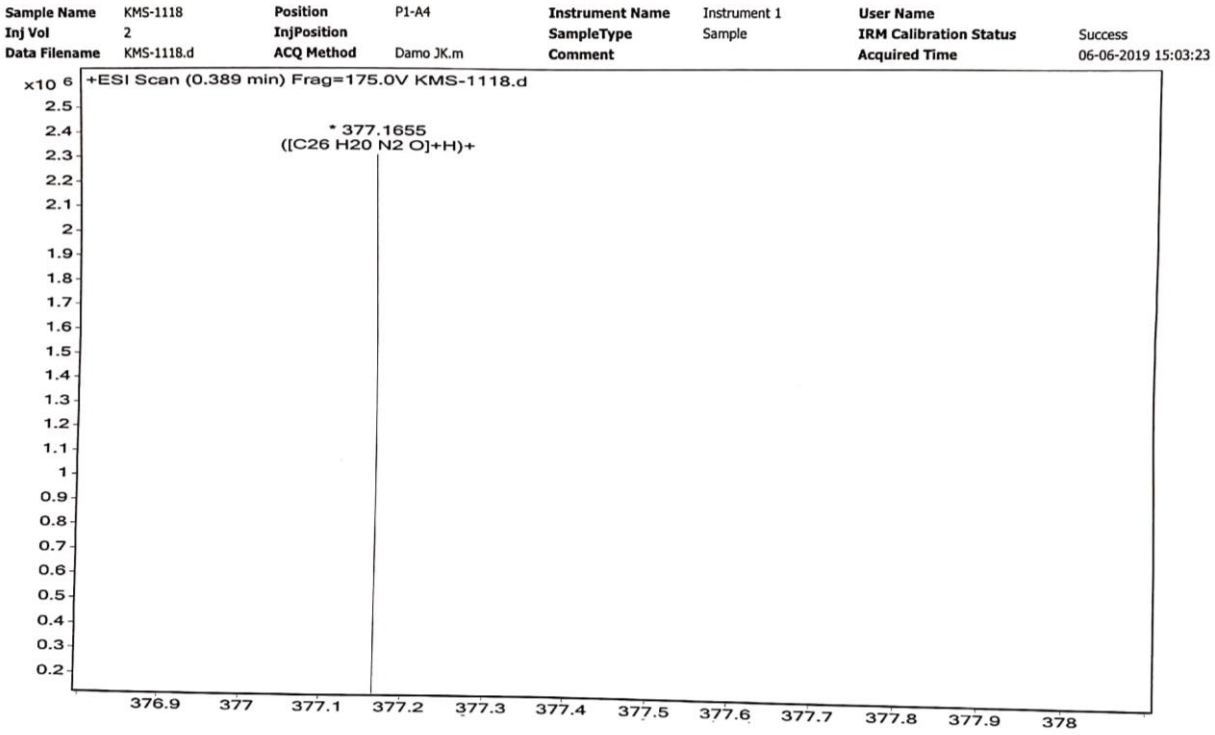




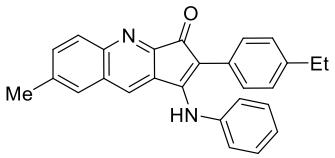
HRMS



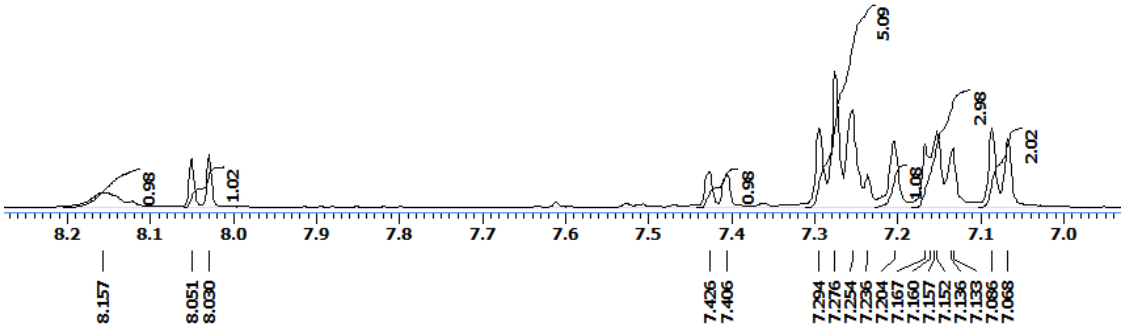
7-Methyl-1-(phenylamino)-2-(*o*-tolyl)-3*H*-cyclopenta[b]quinolin-3-one (3k)

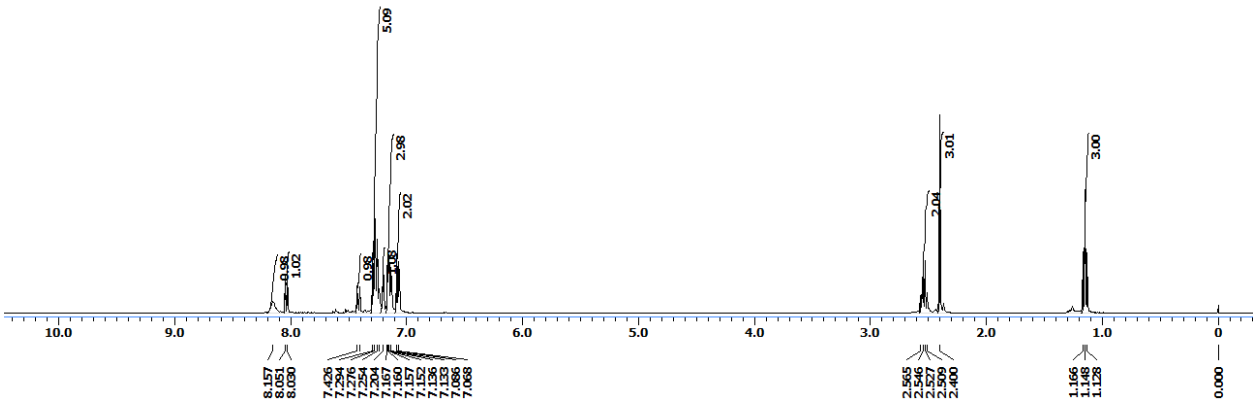


^{1}H NMR

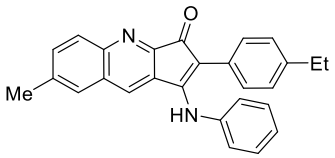


2-(4-Ethylphenyl)-7-methyl-1-(phenylamino)-3*H*-cyclopenta[b]quinolin-3-one (3l)

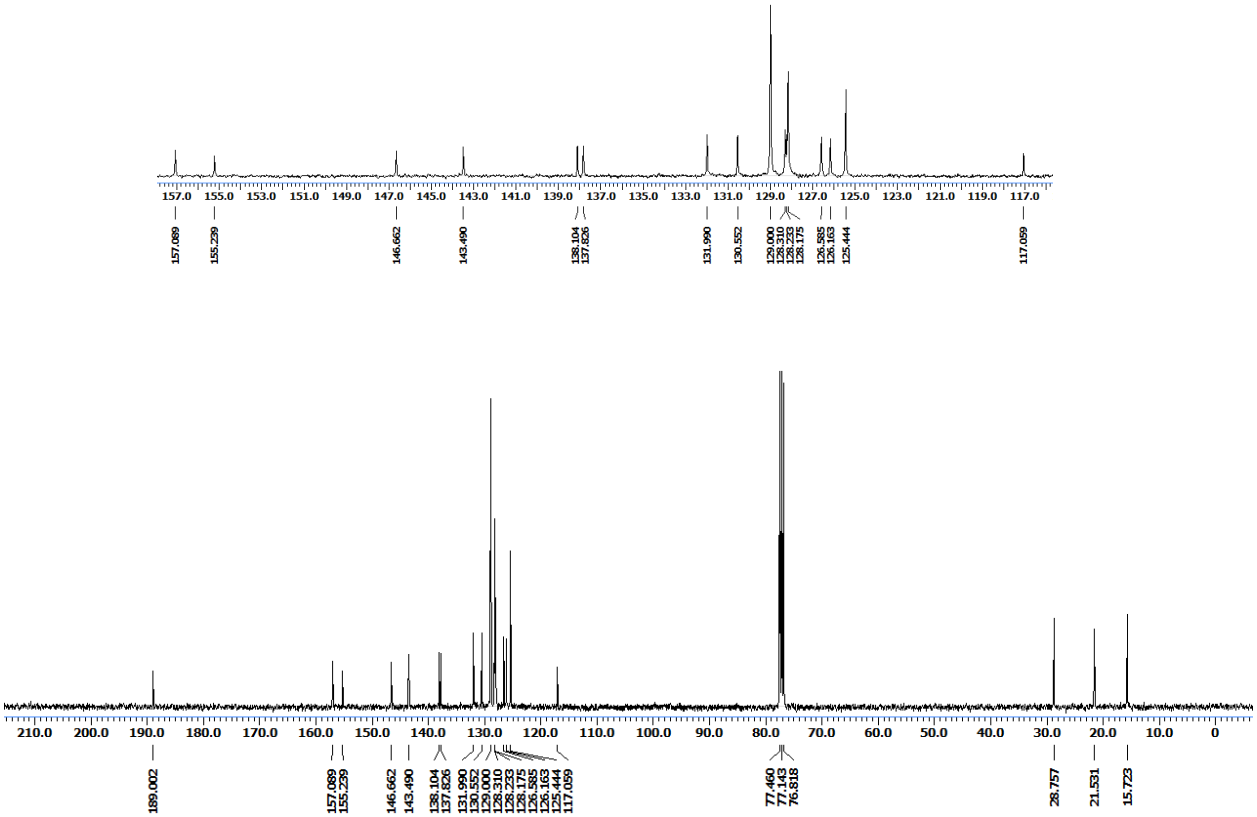




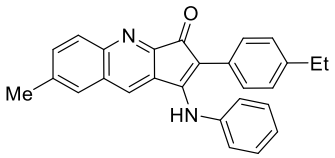
^{13}C NMR



2-(4-Ethylphenyl)-7-methyl-1-(phenylamino)-3*H*-cyclopenta[b]quinolin-3-one (3l)



HRMS



2-(4-Ethylphenyl)-7-methyl-1-(phenylamino)-3*H*-cyclopenta[b]quinolin-3-one (3l)

Qualitative Compound Report

Data File	KMS-1111.d	**Sample Name**	KMS-1111
Sample Type	Sample	**Position**	P1-A2
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	30-05-2019 12:09:07
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

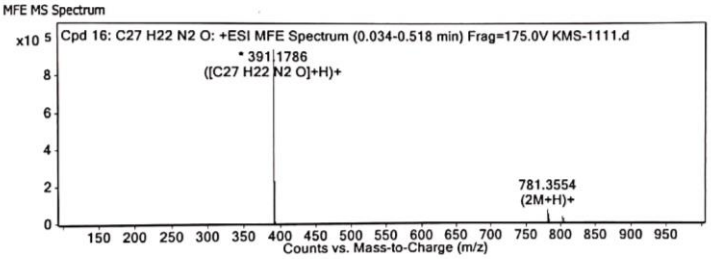
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

Compound Table

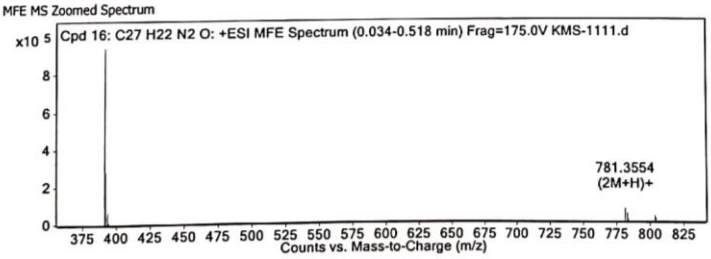
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 16: C27 H22 N2 O	0.11	390.1717	C27 H22 N2 O	C27 H22 N2 O	4	C27 H22 N2 O

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 16: C27 H22 N2 O	391.1786	0.11	Find by Molecular Feature	390.1717

MFE MS Spectrum



MFE MS Zoomed Spectrum

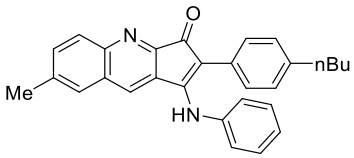


MS Spectrum Peak List

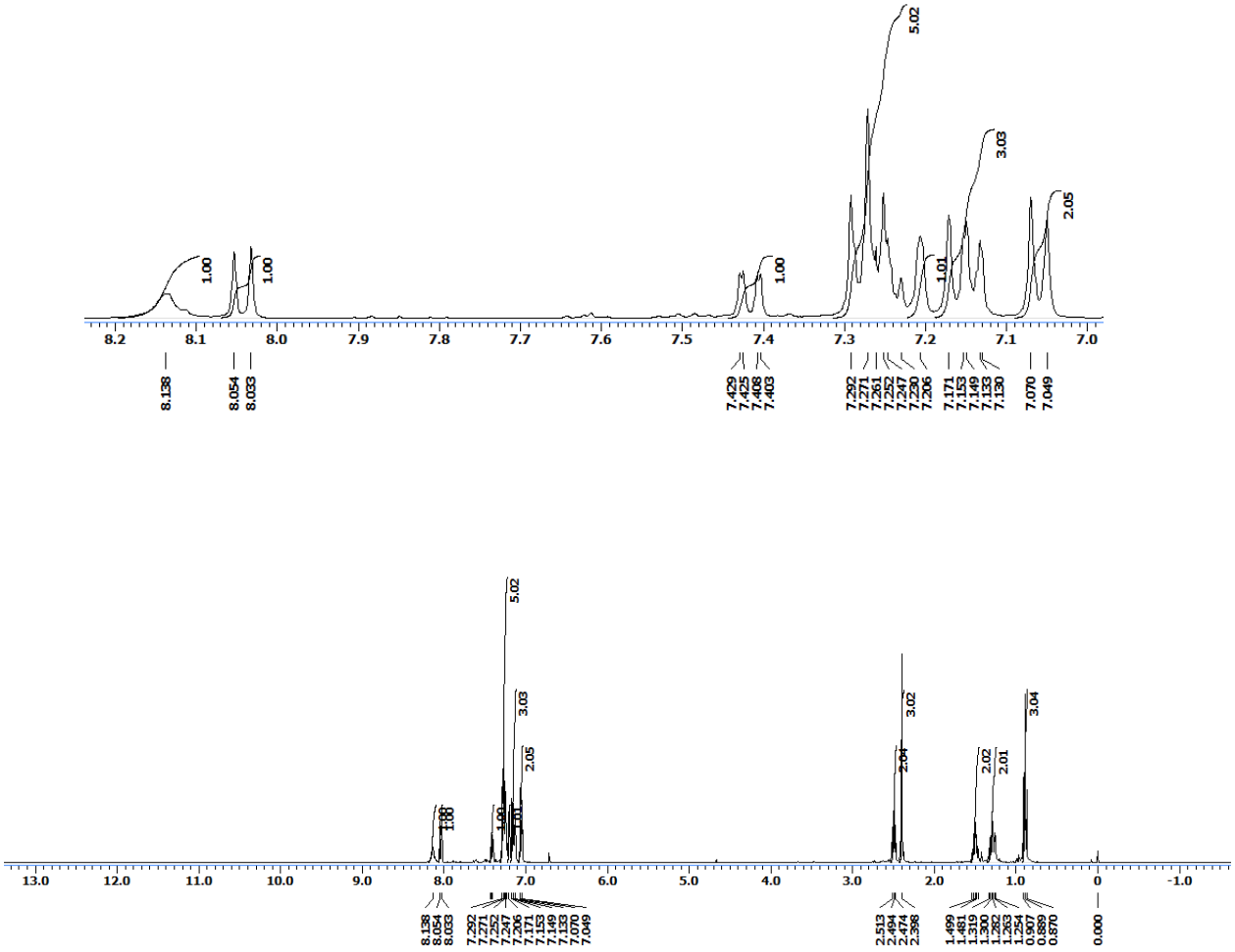
m/z	z	Abund	Formula	Ion
391.1786	1	943206.13	C27 H22 N2 O	(M+H)+
392.182	1	227367.54	C27 H22 N2 O	(M+H)+
393.1902	1	63149.29	C27 H22 N2 O	(M+H)+
394.1944	1	10057.86	C27 H22 N2 O	(M+H)+
781.3554	1	70017.52		(2M+H)+
782.3594	1	44262.72		(2M+H)+
783.3644	1	15725.35		(2M+H)+
803.3357	1	30654.54		(2M+Na)+
804.3392	1	20013.9		(2M+Na)+
805.345	1	6648.76		(2M+Na)+

--- End Of Report ---

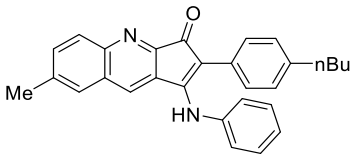
^{1}H NMR



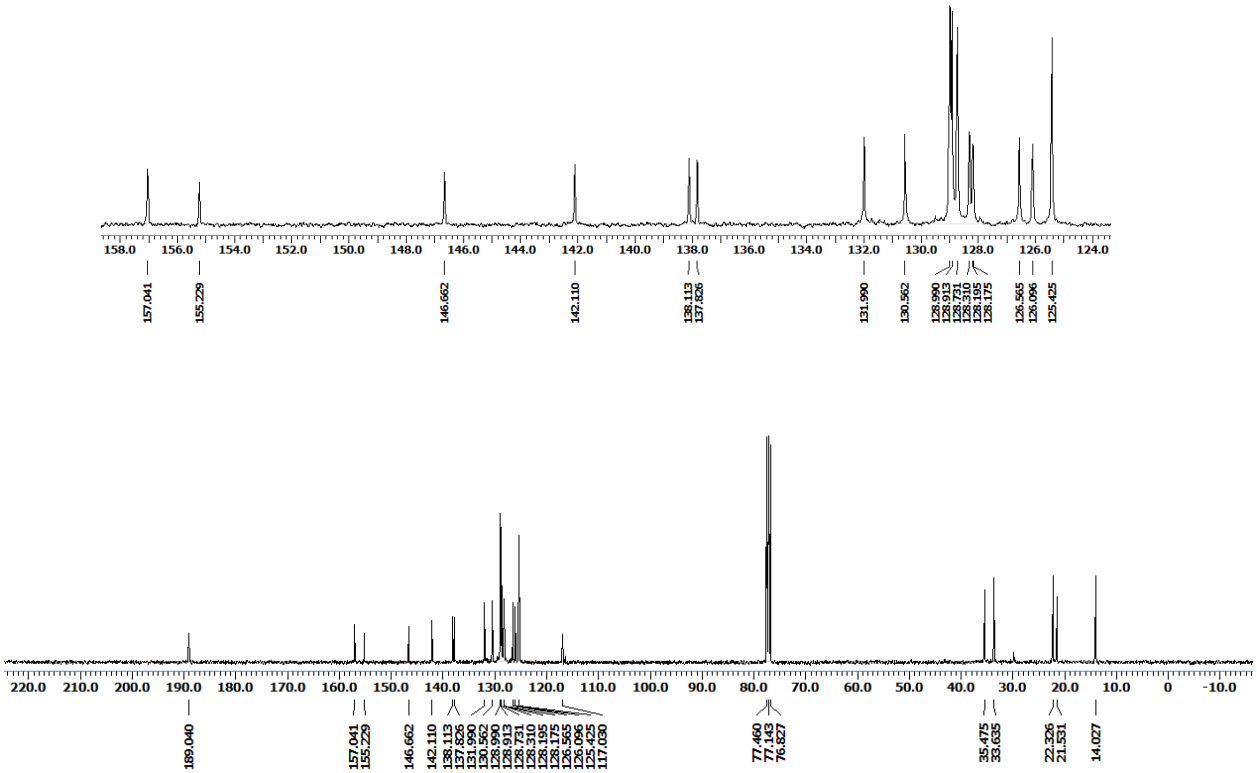
2-(4-Butylphenyl)-7-methyl-1-(phenylamino)-3*H*-cyclopenta[b]quinolin-3-one (3m)



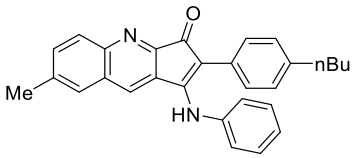
^{13}C NMR



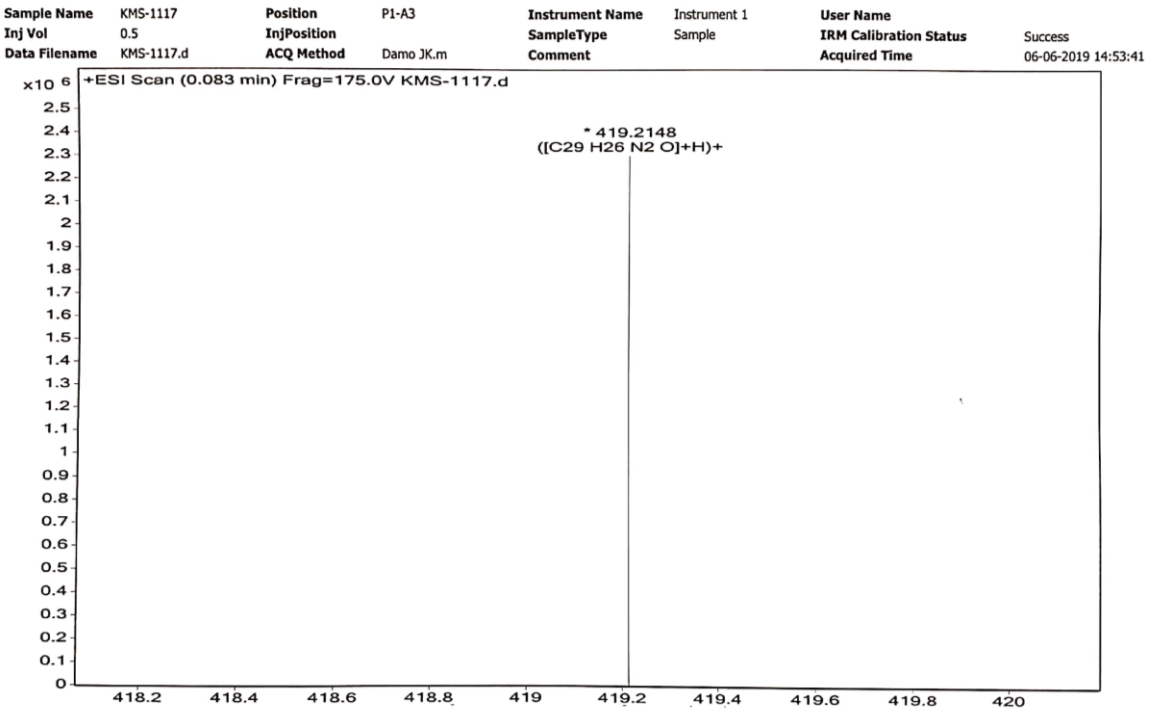
2-(4-Butylphenyl)-7-methyl-1-(phenylamino)-3*H*-cyclopenta[b]quinolin-3-one (3m)



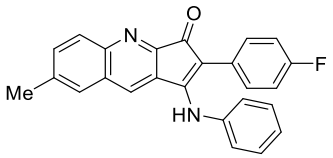
HRMS



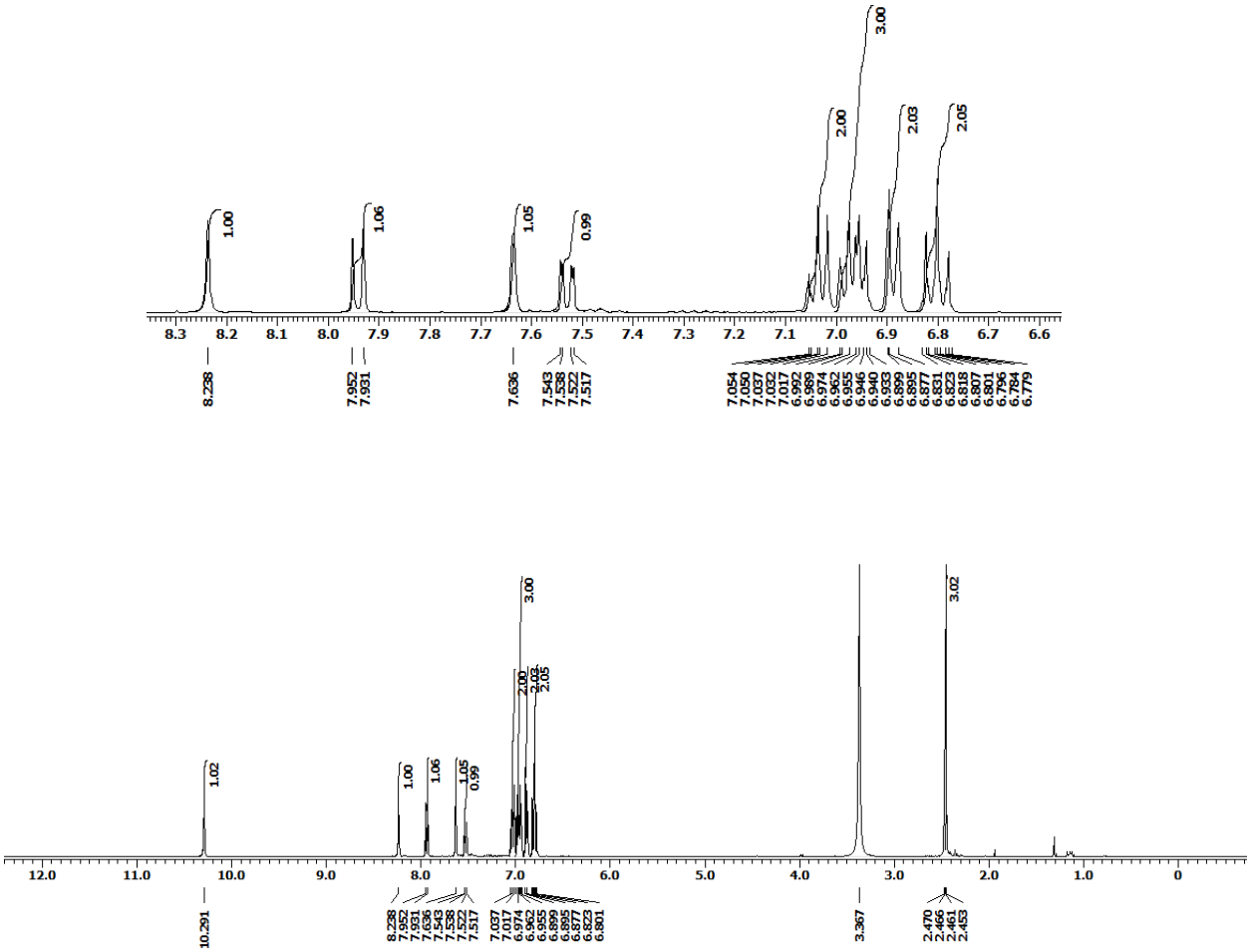
2-(4-Butylphenyl)-7-methyl-1-(phenylamino)-3*H*-cyclopenta[b]quinolin-3-one (3m)



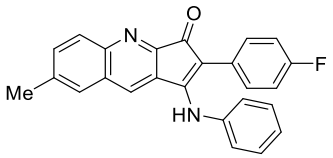
^{1}H NMR



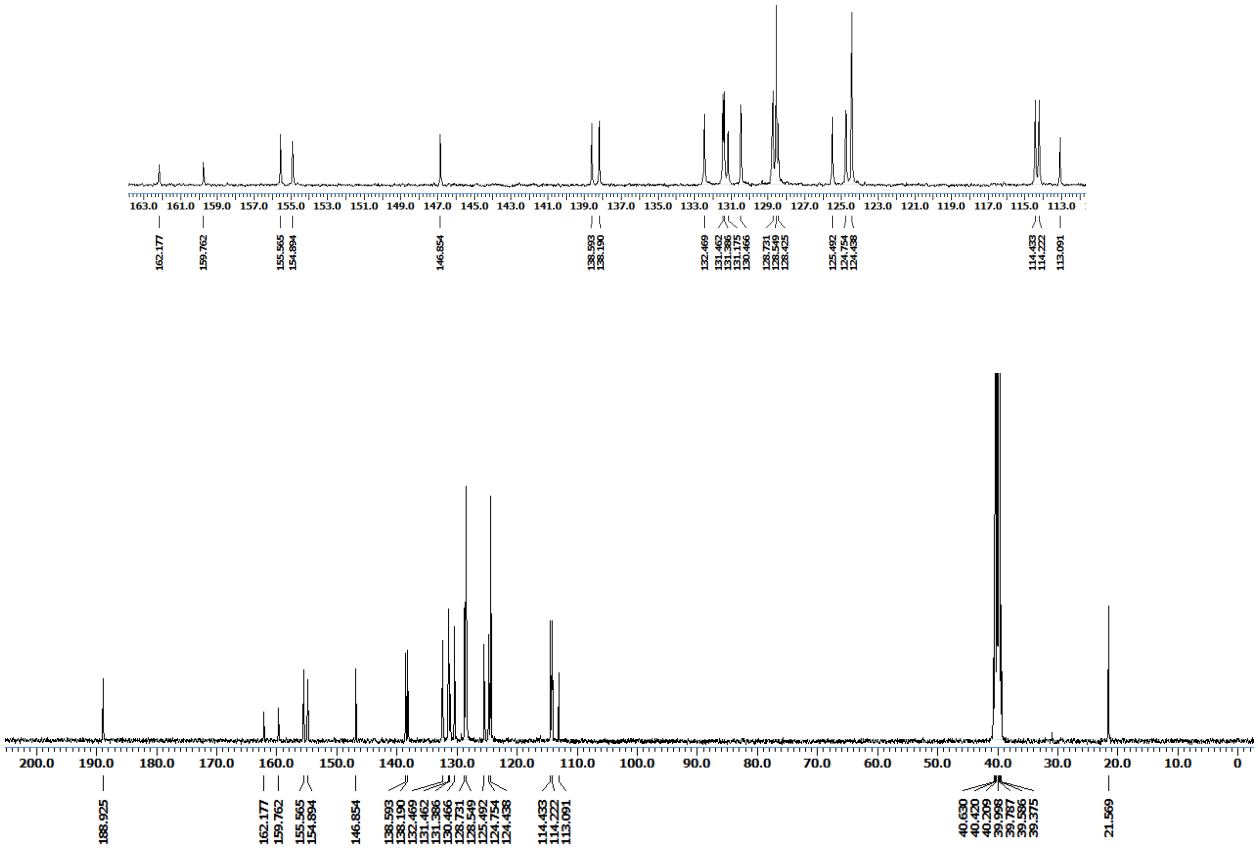
2-(4-Fluorophenyl)-7-methyl-1-(phenylamino)-3*H*-cyclopenta[b]quinolin-3-one (3n)



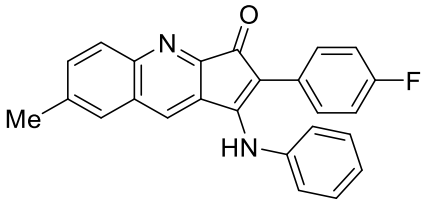
^{13}C NMR



2-(4-Fluorophenyl)-7-methyl-1-(phenylamino)-3*H*-cyclopenta[b]quinolin-3-one (3n)



HRMS



2-(4-Fluorophenyl)-7-methyl-1-(phenylamino)-3*H*-cyclopenta[b]quinolin-3-one (3n)

Qualitative Compound Report

Data File	KMS-1132.d	**Sample Name**	KMS-1132
Sample Type	Sample	**Position**	P1-A7
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	20-06-2019 09:55:27
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

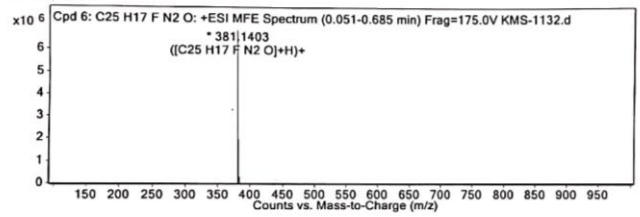
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

Compound Table

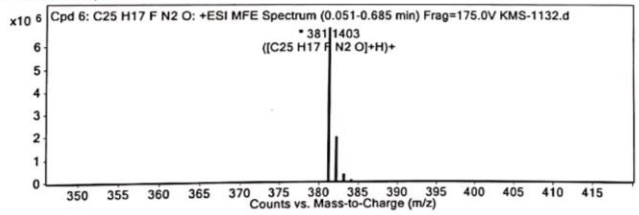
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 6: C25 H17 F N2 O	0.11	380.1331	C25 H17 F N2 O	C25 H17 F N2 O	-1.47	C25 H17 F N2 O

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 6: C25 H17 F N2 O	381.1403	0.11	Find by Molecular Feature	380.1331

MFE MS Spectrum



MFE MS Zoomed Spectrum

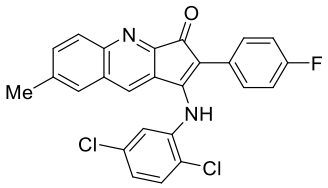


MS Spectrum Peak List

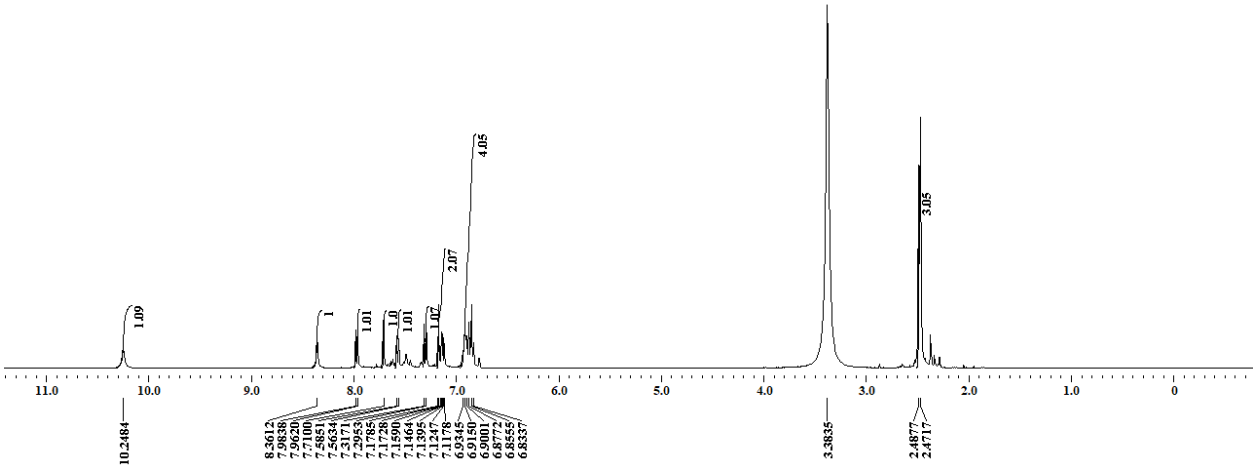
m/z	z	Abund	Formula	Ion
381.1403	1	6864446	C25 H17 F N2 O	(M+H)+
382.1436	1	1969383.6	C25 H17 F N2 O	(M+H)+
383.1467	1	266489.74	C25 H17 F N2 O	(M+H)+
384.1498	1	28491.53	C25 H17 F N2 O	(M+H)+
385.1436	1	3277.24	C25 H17 F N2 O	(M+H)+

--- End Of Report ---

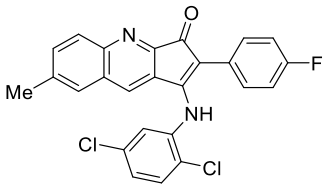
^{1}H NMR



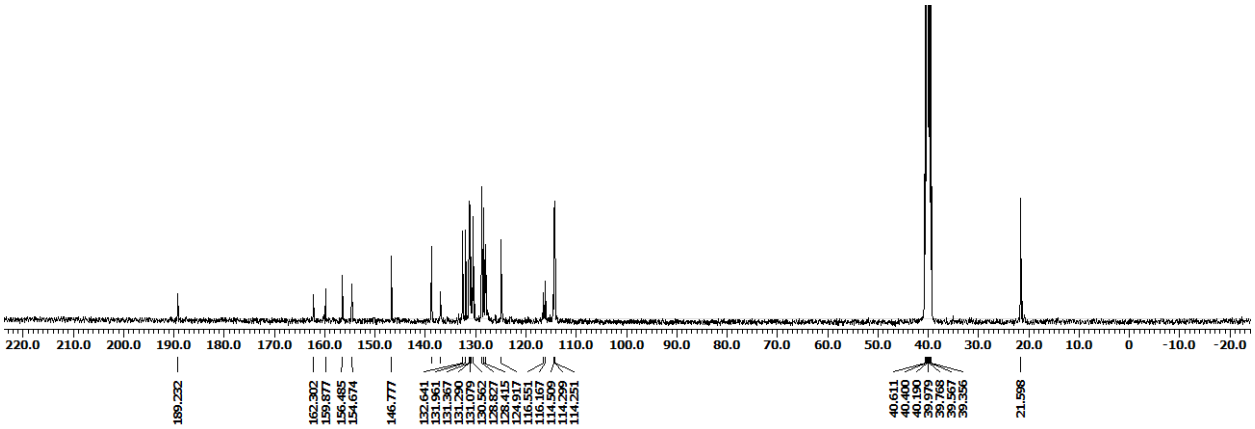
1-((2, 5-Dichlorophenyl) amino)-2-(4-fluorophenyl)-7-methyl-3*H*-cyclopenta[b]quinolin-3-one (3o)



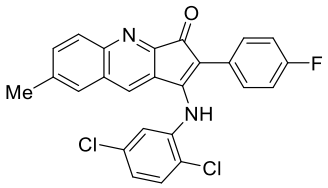
^{13}C NMR



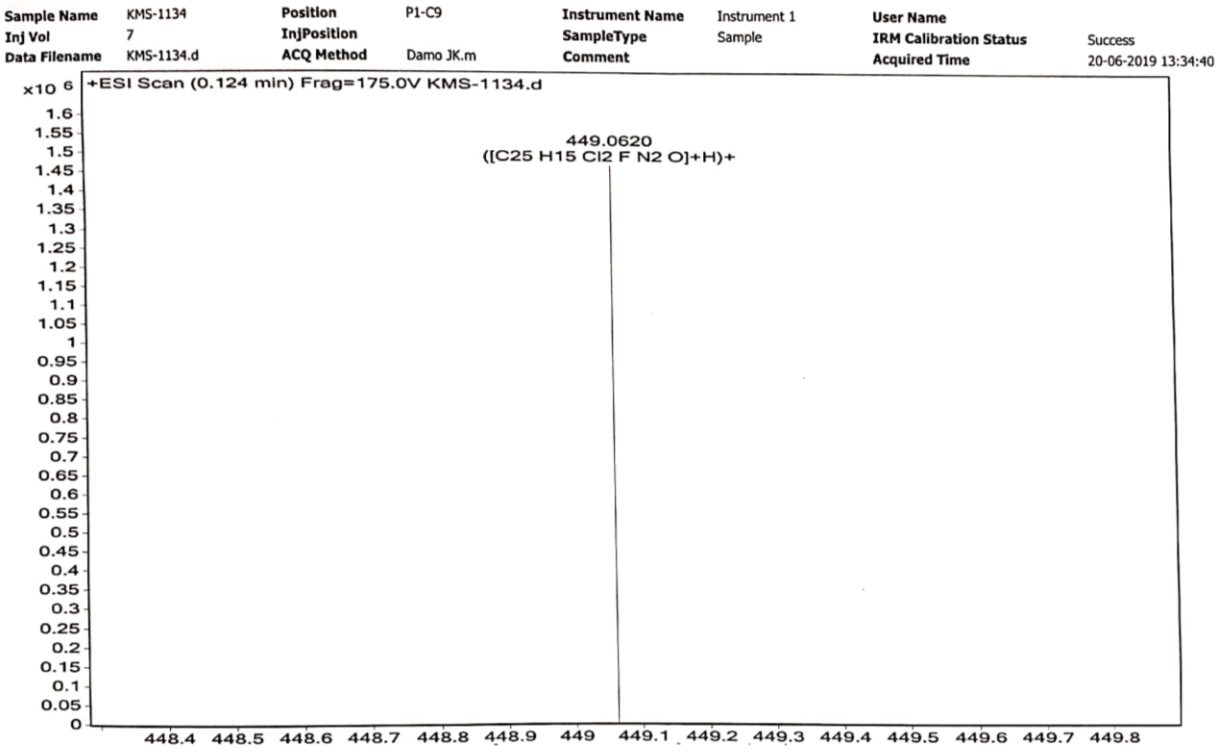
1-((2,5-Dichlorophenyl) amino)-2-(4-fluorophenyl)-7-methyl-3*H*-cyclopenta[b]quinolin-3-one (3o)



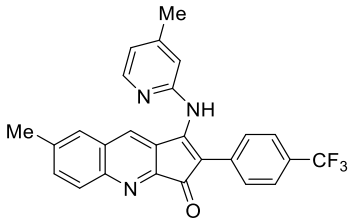
HRMS



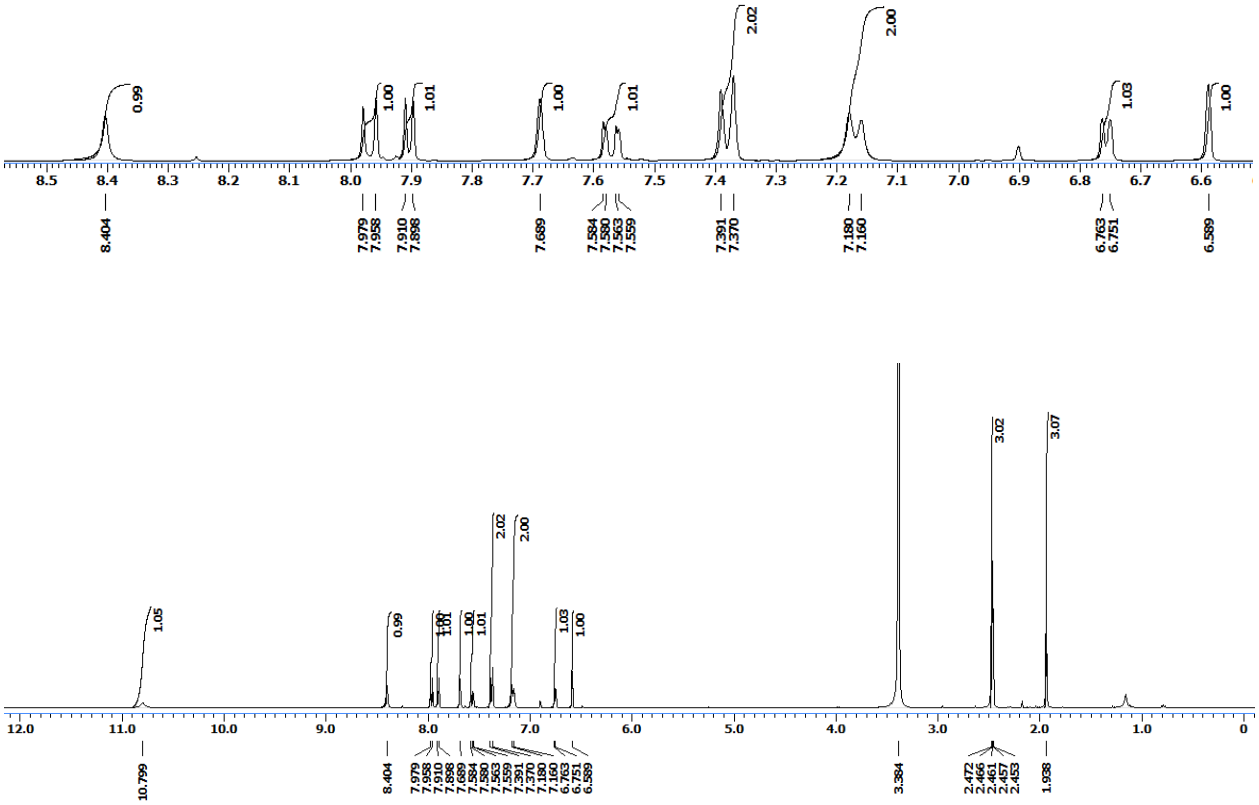
1-((2,5-Dichlorophenyl) amino)-2-(4-fluorophenyl)-7-methyl-3*H*-cyclopenta[b]quinolin-3-one (3o)



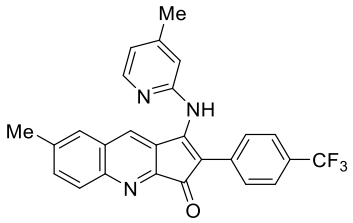
^{1}H NMR



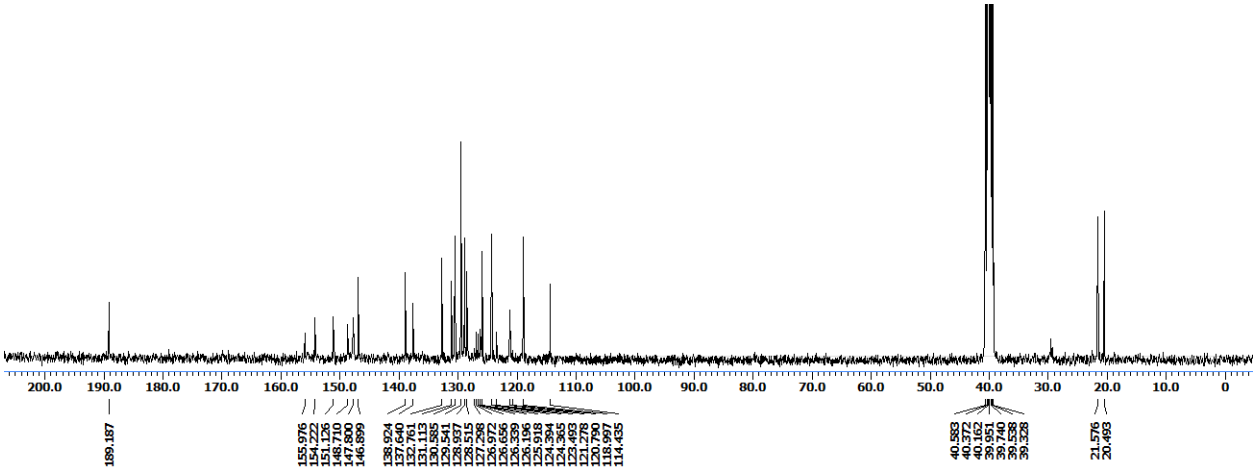
7-Methyl-1-((4-methylpyridin-2-yl)amino)-2-(4-(trifluoromethyl)phenyl)-3*H*-cyclopenta[b]quinolin-3-one (3p)



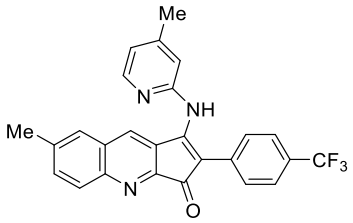
^{13}C NMR



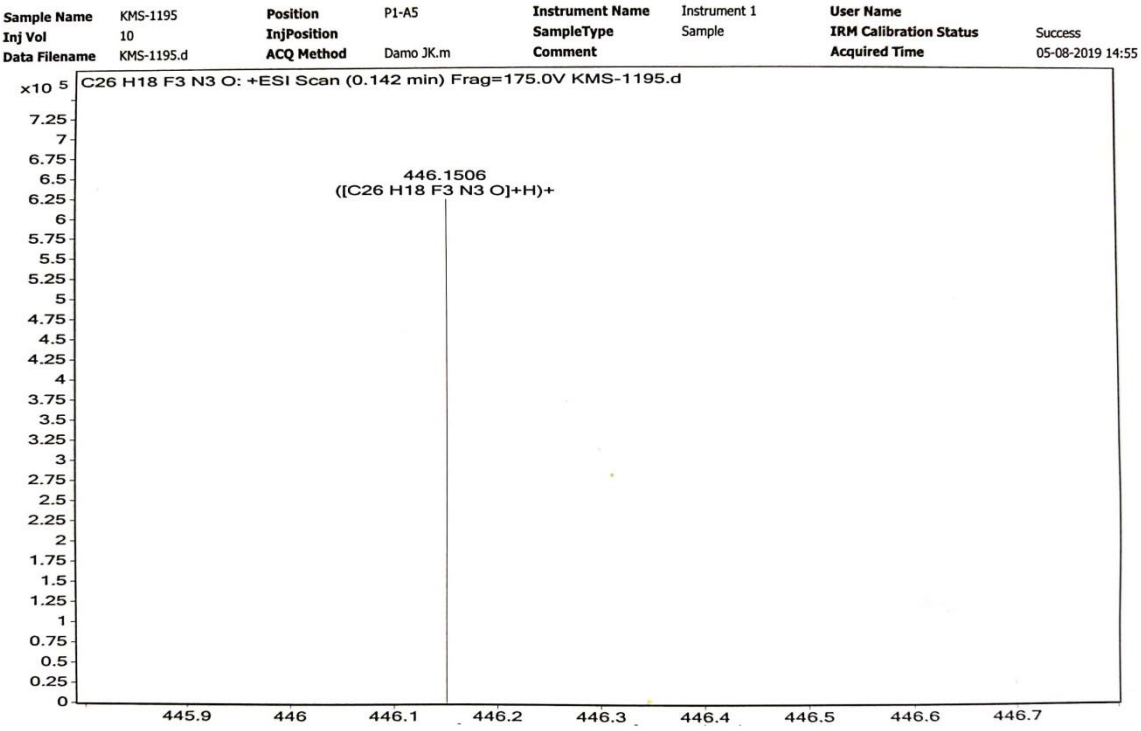
7-Methyl-1-((4-methylpyridin-2-yl)amino)-2-(4-(trifluoromethyl)phenyl)-3*H*-cyclopenta[b]quinolin-3-one (3p)



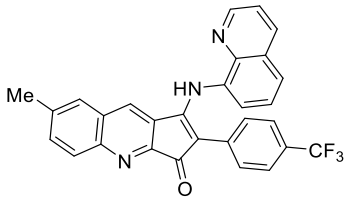
HRMS



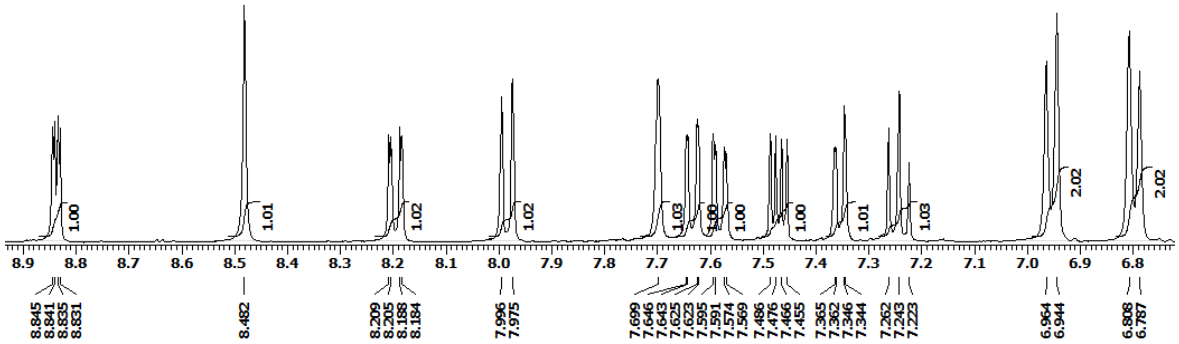
7-Methyl-1-((4-methylpyridin-2-yl)amino)-2-(4-(trifluoromethyl)phenyl)-3*H*-cyclopenta[b]quinolin-3-one (3p)

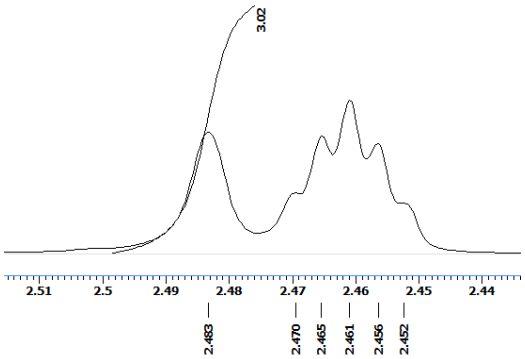


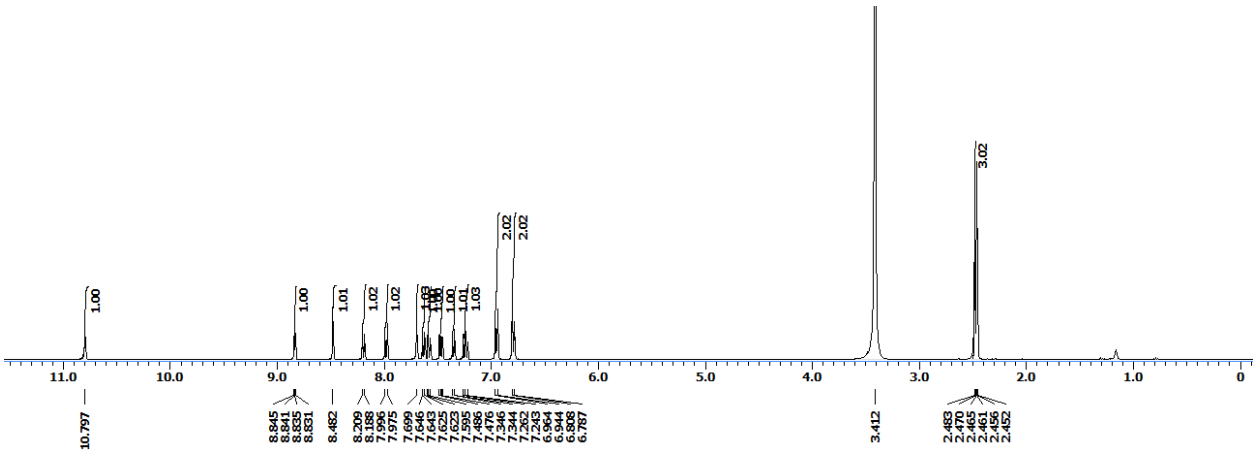
^{1}H NMR



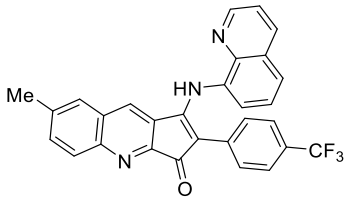
7-Methyl-1-(quinolin-8-ylamino)-2-(4-(trifluoromethyl)phenyl)-3*H*-cyclopenta[b]quinolin-3-one (3q)



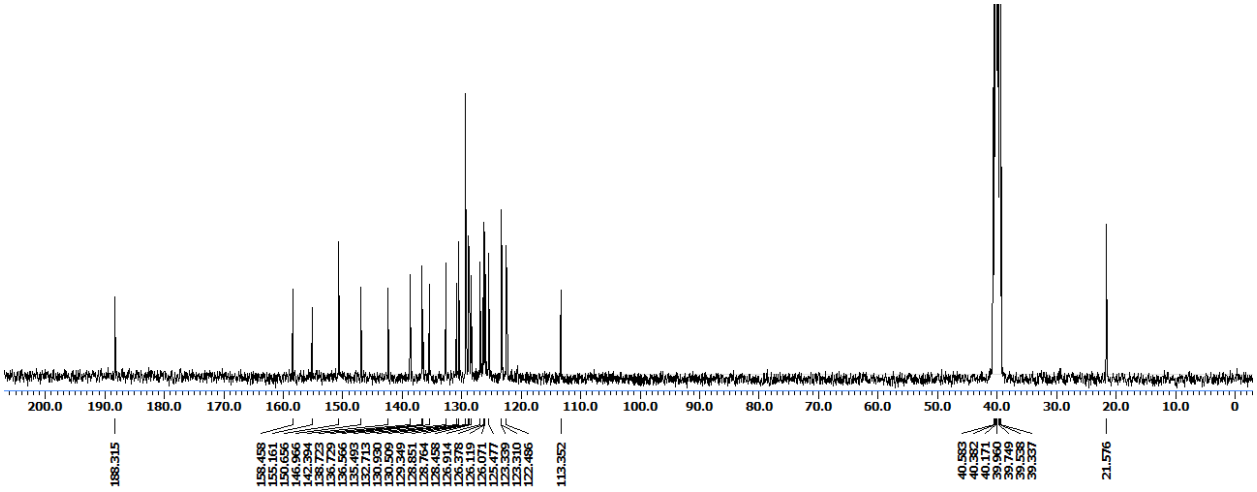




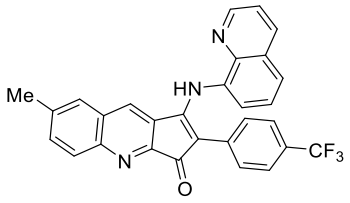
^{13}C NMR



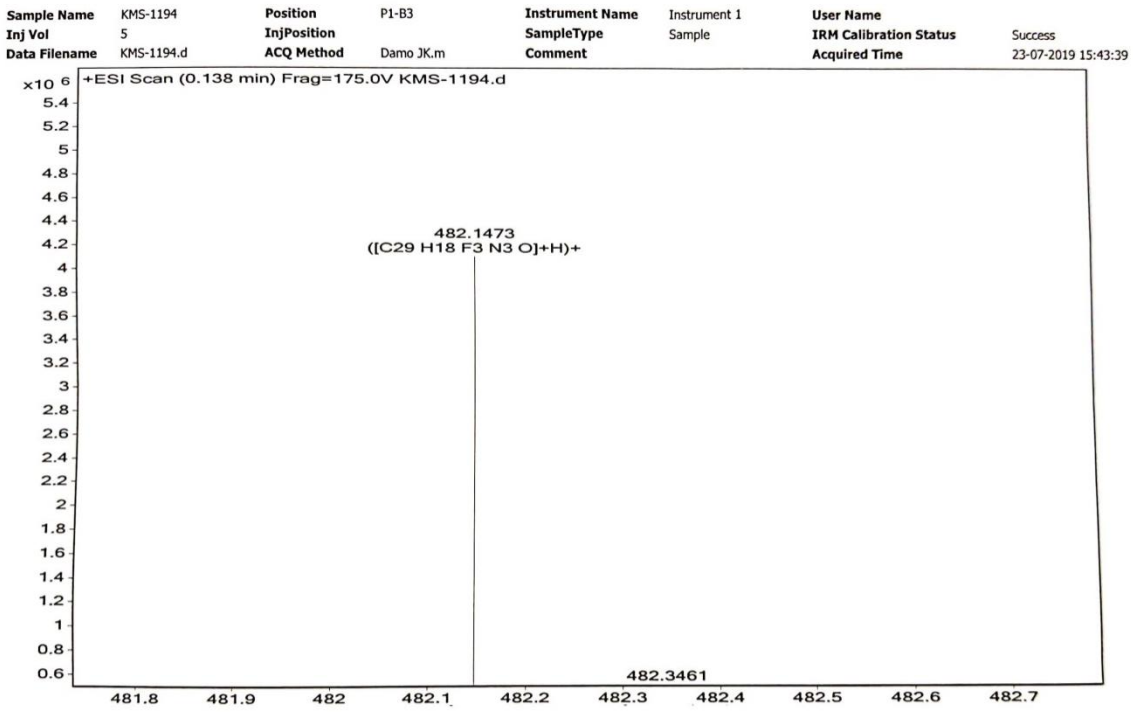
7-Methyl-1-(quinolin-8-ylamino)-2-(4-(trifluoromethyl)phenyl)-3*H*-cyclopenta[b]quinolin-3-one (3q)



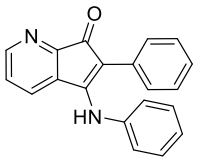
HRMS



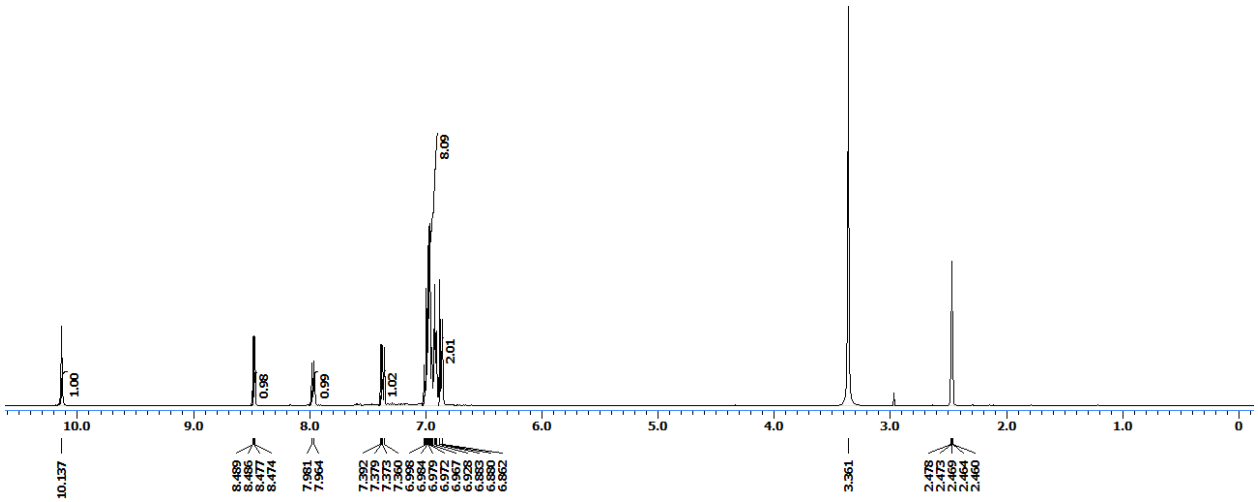
7-Methyl-1-(quinolin-8-ylamino)-2-(4-(trifluoromethyl)phenyl)-3*H*-cyclopenta[b]quinolin-3-one (3q)



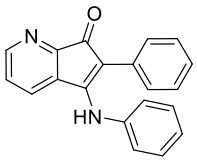
^{1}H NMR



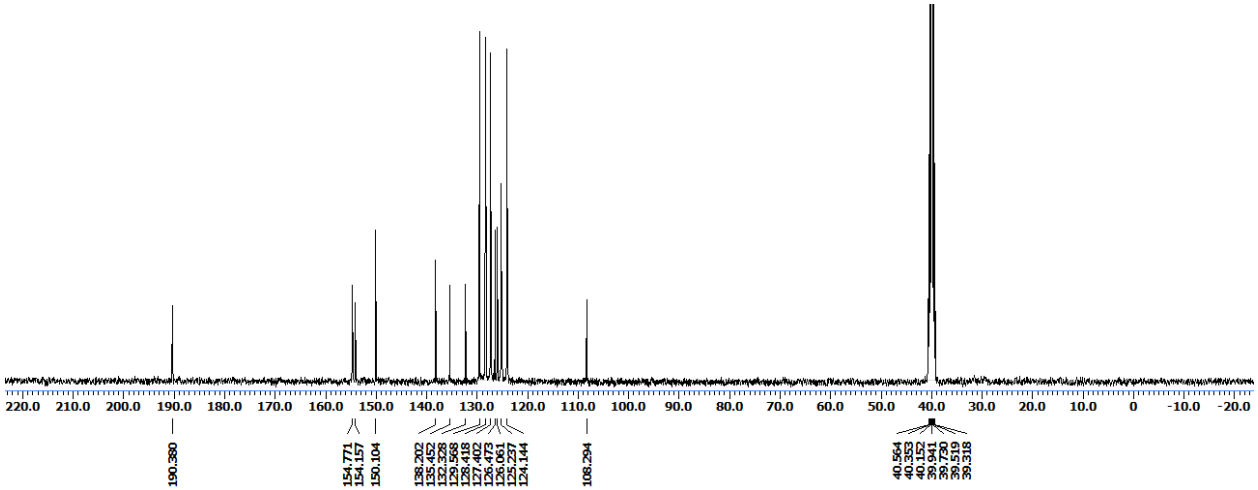
6-Phenyl-5-(phenylamino)-7*H*-cyclopenta[b]pyridin-7-one (5a)



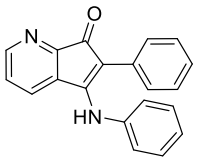
^{13}C NMR



6-Phenyl-5-(phenylamino)-7*H*-cyclopenta[b]pyridin-7-one (5a)



HRMS



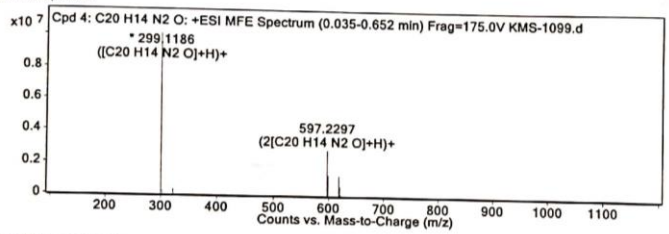
6-Phenyl-5-(phenylamino)-7*H*-cyclopenta[b]pyridin-7-one (5a)

Compound Table

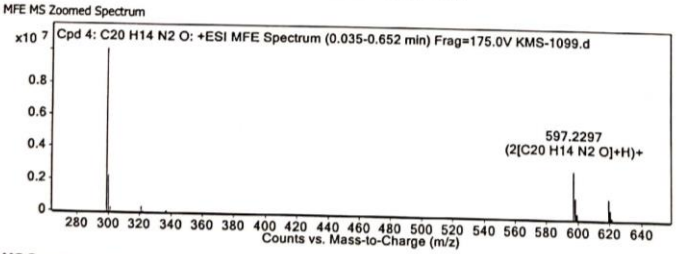
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 4: C20 H14 N2 O	0.098	298.1113	C20 H14 N2 O	C20 H14 N2 O	-2.35	C20 H14 N2 O

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 4: C20 H14 N2 O	299.1186	0.098	Find by Molecular Feature	298.1113

MFE MS Spectrum



MFE MS Zoomed Spectrum

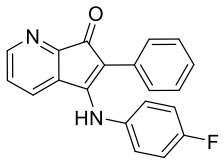


MS Spectrum Peak List

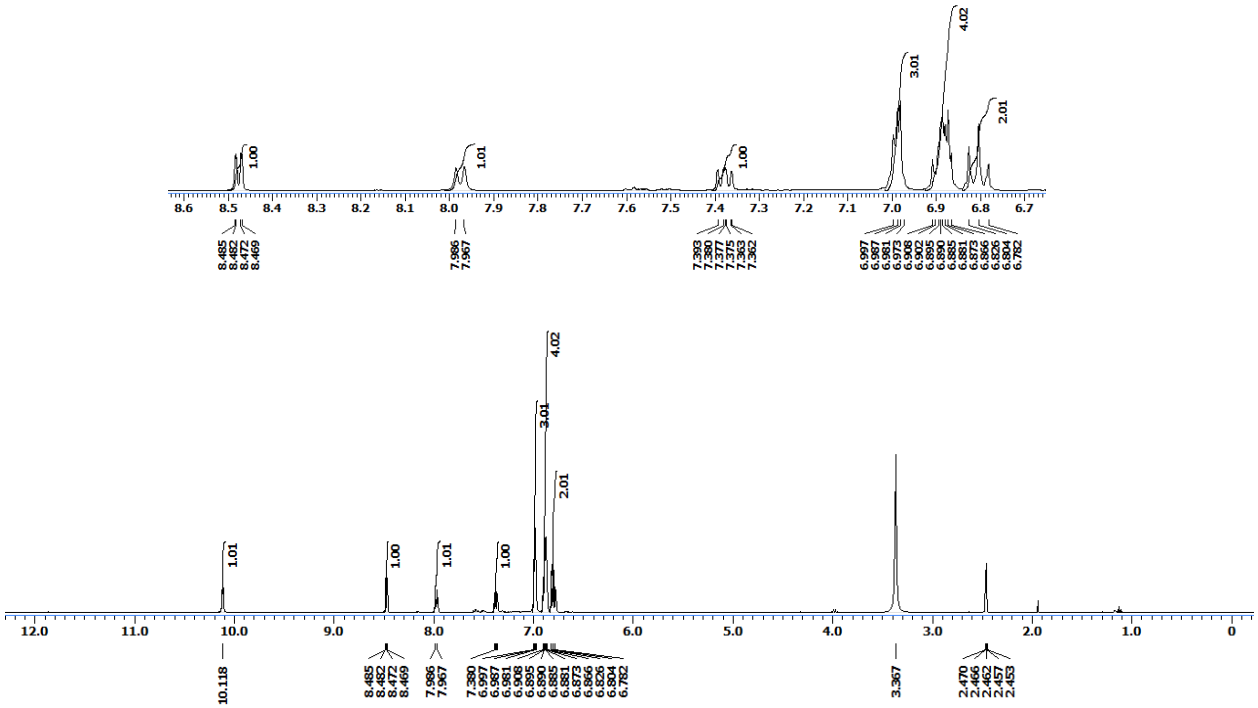
m/z	z	Abund	Formula	Ion
299.1186	1	10115842	C20 H14 N2 O	(M+H)+
300.1219	1	2216810.59	C20 H14 N2 O	(M+H)+
301.1251	1	183964.92	C20 H14 N2 O	(M+H)+
321.1005	1	303277.56	C20 H14 N2 O	(M+Na)+
597.2297	1	2856531.5	C20 H14 N2 O	(2M+H)+
598.2331	1	1319687.81	C20 H14 N2 O	(2M+H)+
599.228	1	346351.15	C20 H14 N2 O	(2M+H)+
619.212	1	1255096.13	C20 H14 N2 O	(2M+Na)+
620.2149	1	564579.11	C20 H14 N2 O	(2M+Na)+
621.2177	1	122149.77	C20 H14 N2 O	(2M+Na)+

--- End Of Report ---

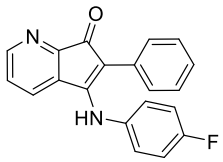
^{1}H NMR



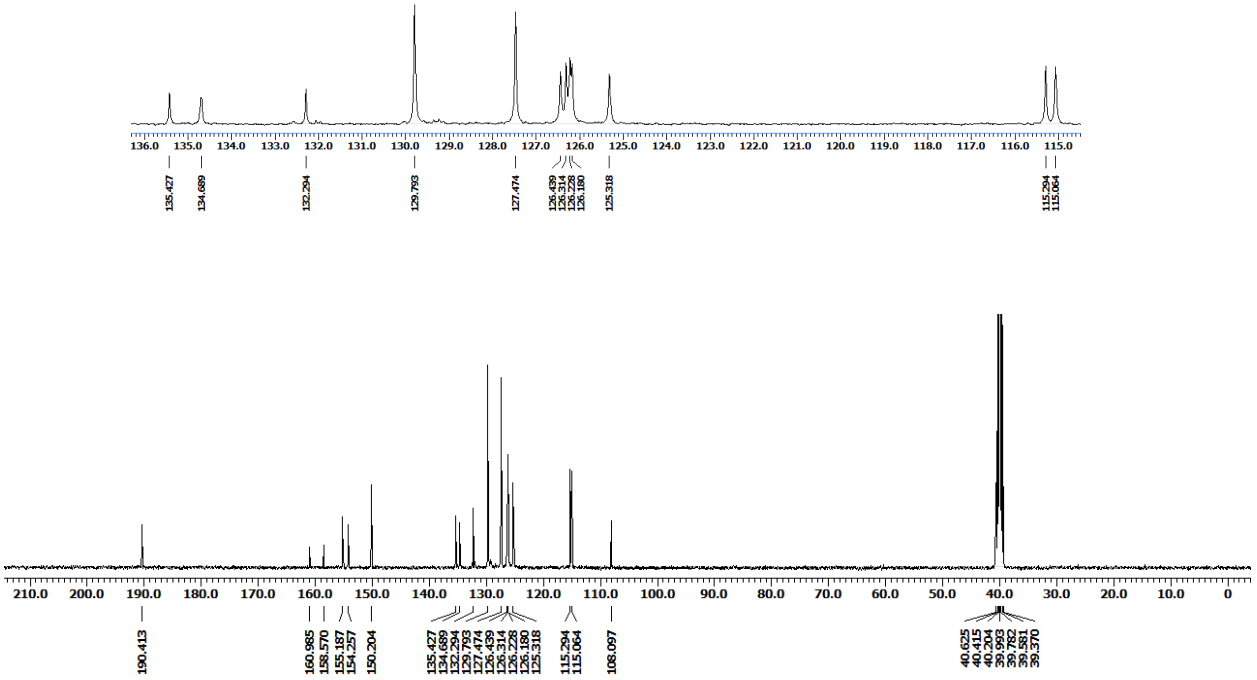
5-((4-Fluorophenyl)amino)-6-phenyl-7*H*-cyclopenta[b]pyridin-7-one (5b)



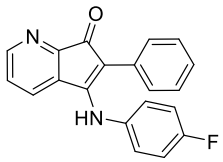
^{13}C NMR



5-((4-Fluorophenyl)amino)-6-phenyl-7*H*-cyclopenta[b]pyridin-7-one (5b)



HRMS



5-((4-Fluorophenyl)amino)-6-phenyl-7*H*-cyclopenta[b]pyridin-7-one (5b)

Qualitative Compound Report

Data File	KMS-1103.d	**Sample Name**	KMS-1103
Sample Type	Sample	**Position**	P1-A3
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	29-05-2019 12:53:52
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

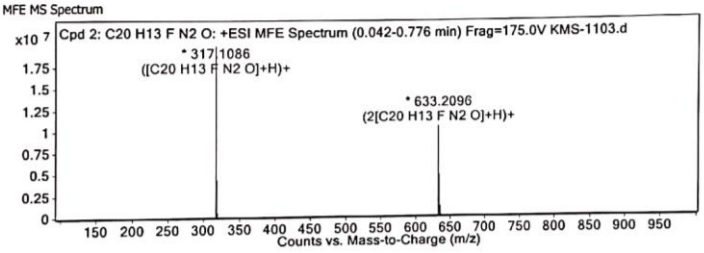
Sample Group **Info.**
Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

Compound Table

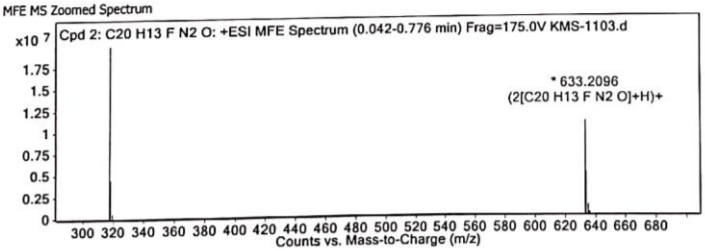
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 2: C20 H13 F N2 O	0.134	316.1012	C20 H13 F N2 O	C20 H13 F N2 O	0.01	C20 H13 F N2 O

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 2: C20 H13 F N2 O	317.1086	0.134	Find by Molecular Feature	316.1012

MFE MS Spectrum



MFE MS Zoomed Spectrum

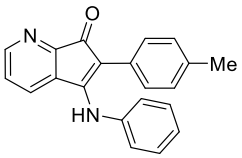


MS Spectrum Peak List

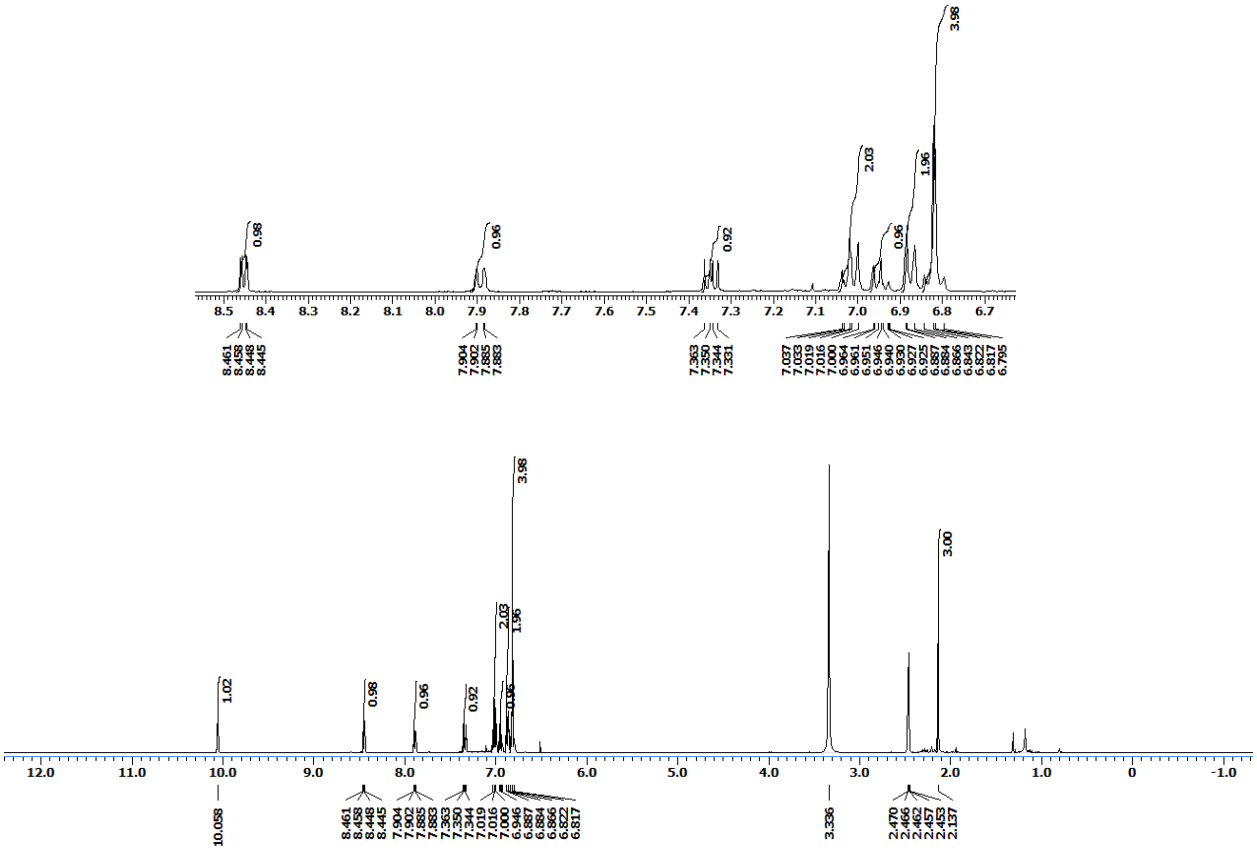
m/z	z	Abund	Formula	Ion
317.1086	1	19971668	C20 H13 F N2 O	(M+H)+
318.1119	1	4351176.33	C20 H13 F N2 O	(M+H)+
319.1151	1	509603.11	C20 H13 F N2 O	(M+H)+
320.118	1	31976.41	C20 H13 F N2 O	(M+H)+
633.2096	1	10605571	C20 H13 F N2 O	(2M+H)+
634.2129	1	4866648.48	C20 H13 F N2 O	(2M+H)+
635.2163	1	1106841.81	C20 H13 F N2 O	(2M+H)+
636.2188	1	169635.85	C20 H13 F N2 O	(2M+H)+
637.2158	1	23467.24	C20 H13 F N2 O	(2M+H)+
671.1664	1	27054.37	C20 H13 F N2 O	(2M+K)+

--- End Of Report ---

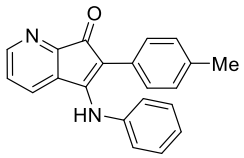
^{1}H NMR



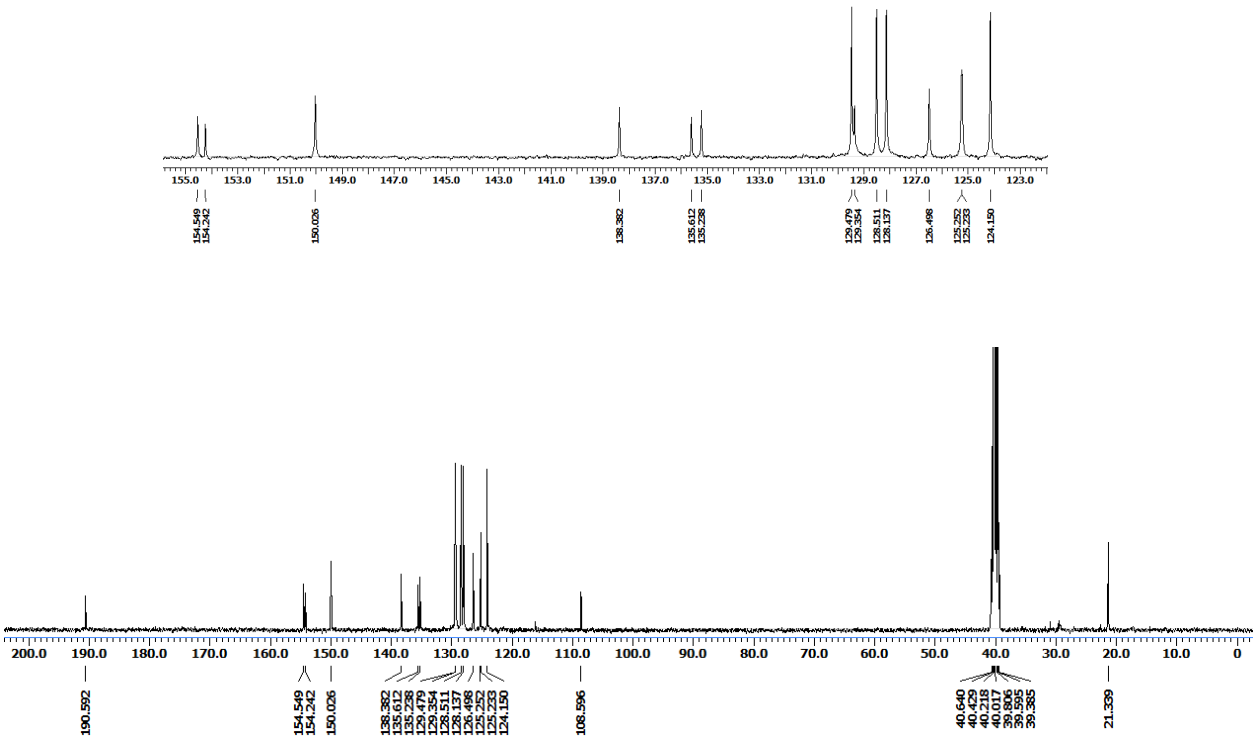
5-(Phenylamino)-6-(*p*-tolyl)-7*H*-cyclopenta[b]pyridin-7-one (5c)



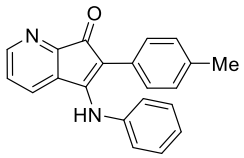
^{13}C NMR



5-(Phenylamino)-6-(*p*-tolyl)-7*H*-cyclopenta[b]pyridin-7-one (5c)



HRMS



5-(Phenylamino)-6-(*p*-tolyl)-7*H*-cyclopenta[b]pyridin-7-one (5c)

Qualitative Compound Report

Data File	KMS-1115.d	**Sample Name**	KMS-1115
Sample Type	Sample	**Position**	P1-A2
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	06-06-2019 14:51:44
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

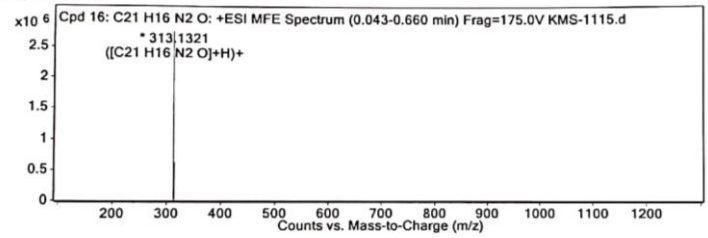
Sample Group **Info.**
Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

Compound Table

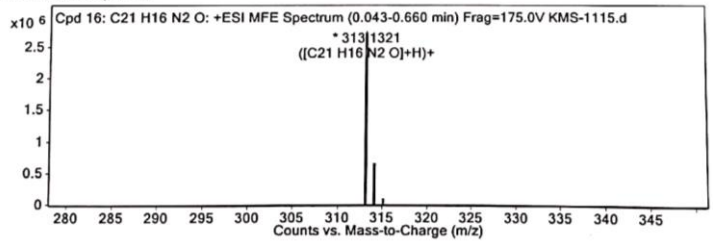
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 16: C21 H16 N2 O	0.109	312.1253	C21 H16 N2 O	C21 H16 N2 O	3.15	C21 H16 N2 O

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 16: C21 H16 N2 O	313.1321	0.109	Find by Molecular Feature	312.1253

MFE MS Spectrum



MFE MS Zoomed Spectrum

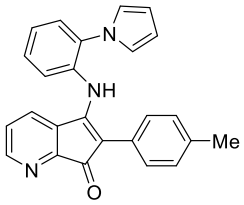


MS Spectrum Peak List

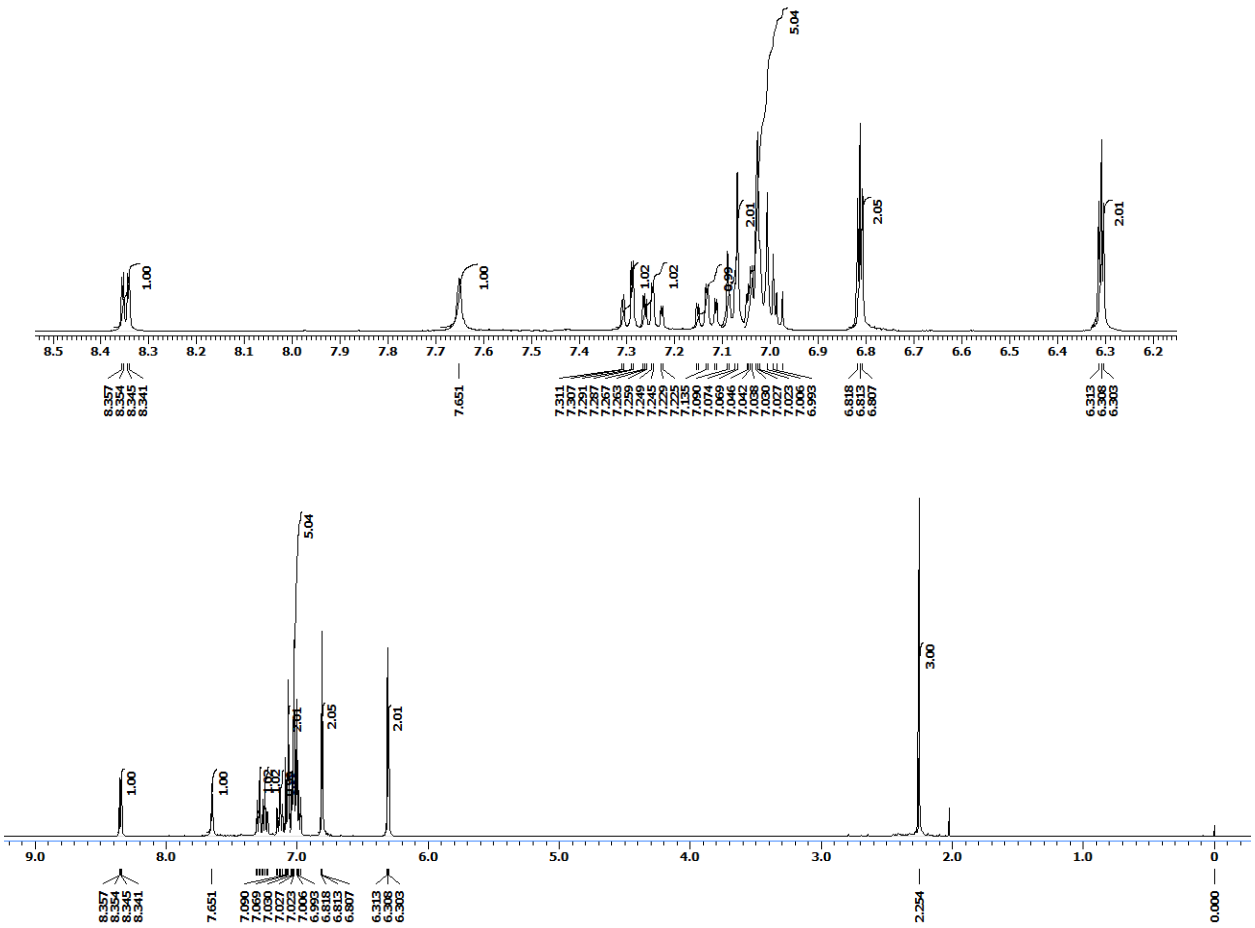
m/z	z	Abund	Formula	Ion
313.1321	1	2756119.5	C21 H16 N2 O	(M+H)+
314.1374	1	621015.07	C21 H16 N2 O	(M+H)+
315.1417	1	69600.77	C21 H16 N2 O	(M+H)+
316.1448	1	2563.82	C21 H16 N2 O	(M+H)+

--- End Of Report ---

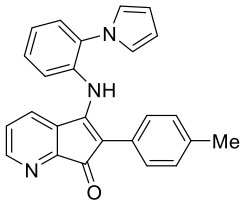
^{1}H NMR



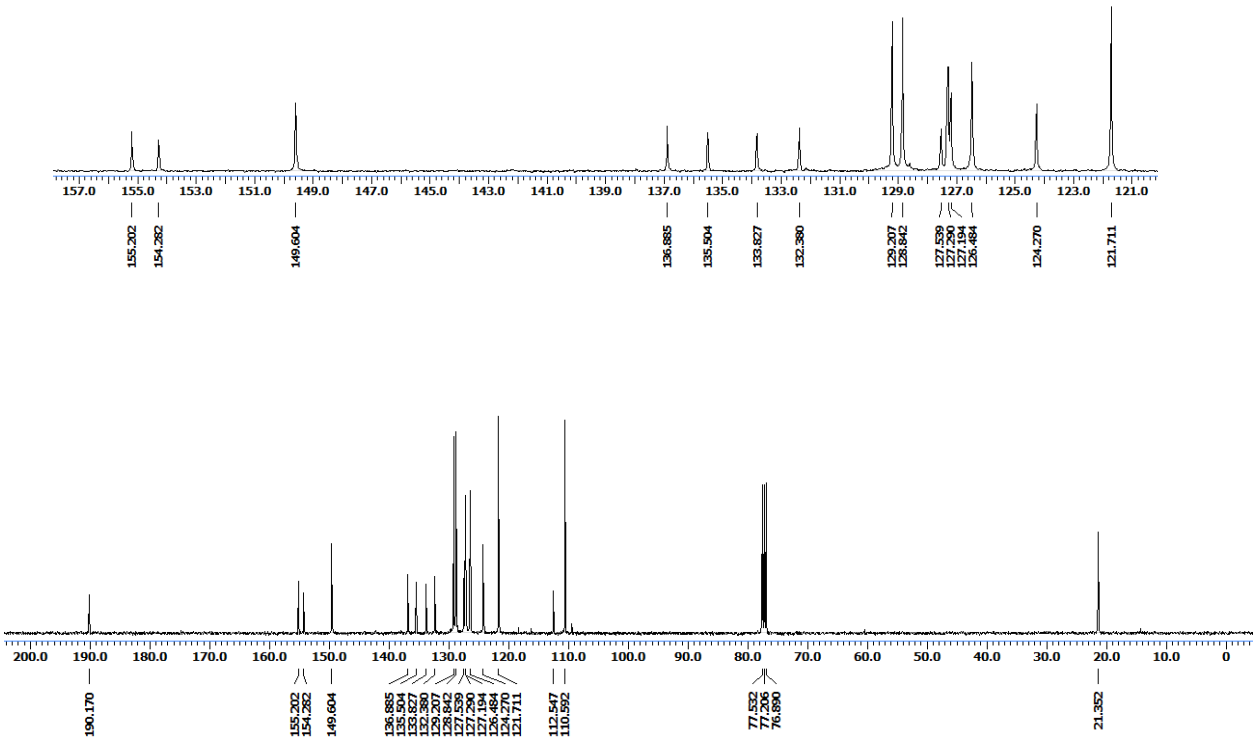
5-((2-(1*H*-pyrrol-1-yl)phenyl)amino)-6-(*p*-tolyl)-7*H*-cyclopenta[b]pyridin-7-one (5d)



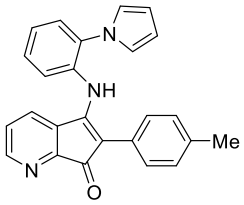
^{13}C NMR



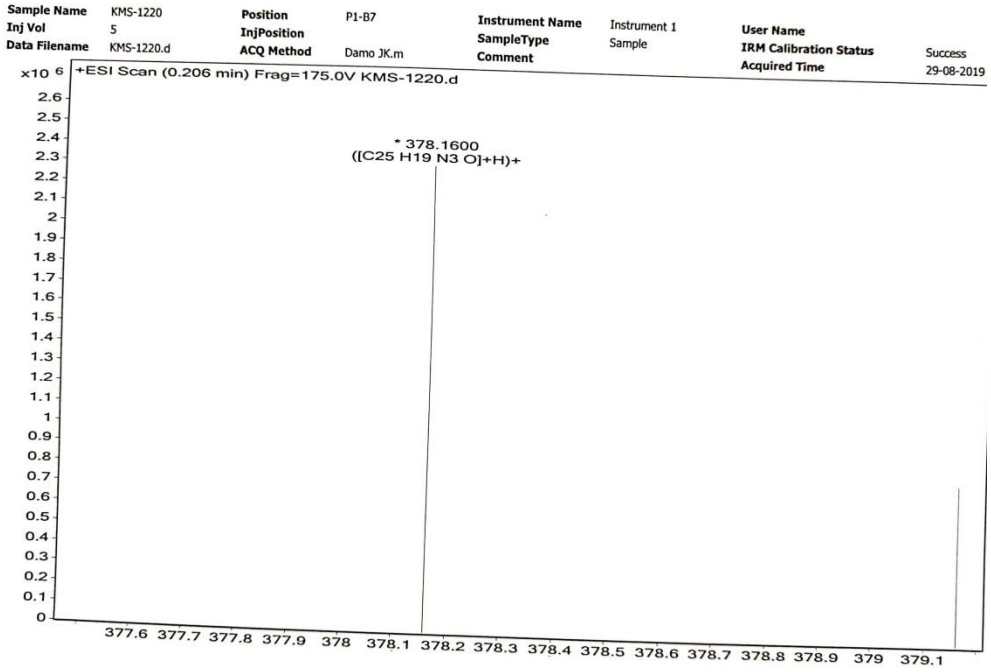
5-((2-(1*H*-pyrrol-1-yl)phenyl)amino)-6-(*p*-tolyl)-7*H*-cyclopenta[b]pyridin-7-one (5d)



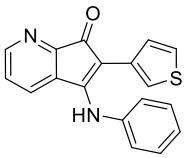
HRMS



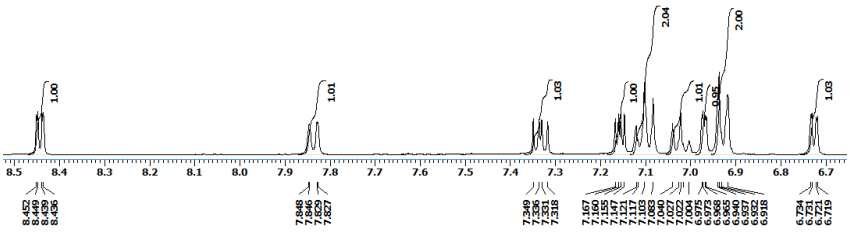
5-((2-(1*H*-pyrrol-1-yl)phenyl)amino)-6-(*p*-tolyl)-7*H*-cyclopenta[b]pyridin-7-one (5d)

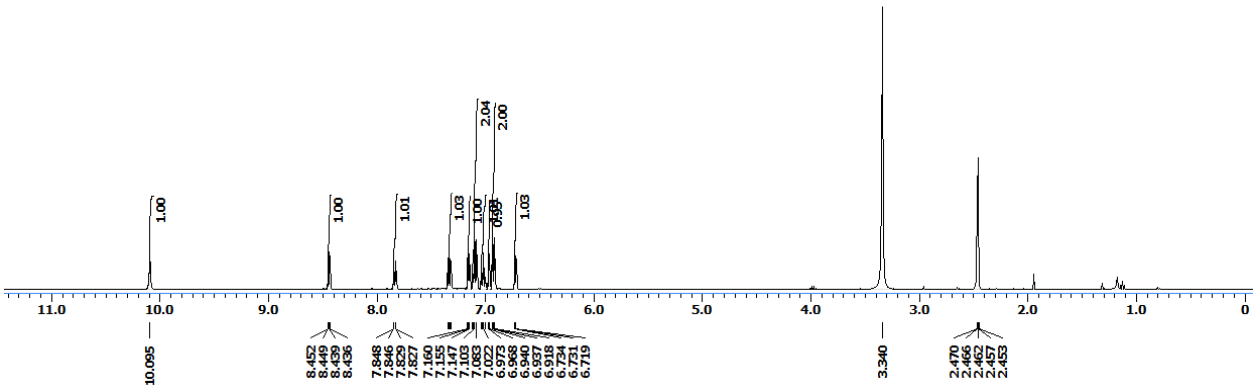


^{1}H NMR

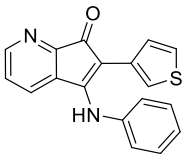


5-(Phenylamino)-6-(thiophen-3-yl)-7*H*-cyclopenta[b]pyridin-7-one (5e)

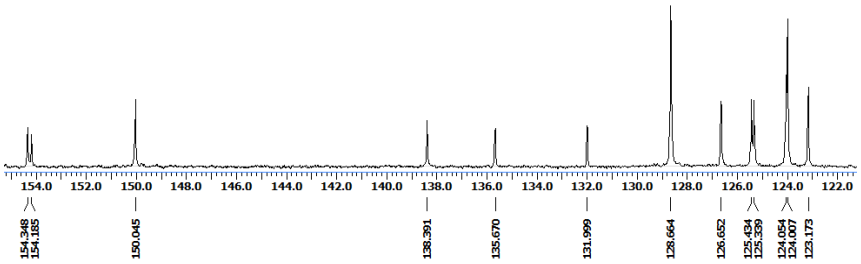


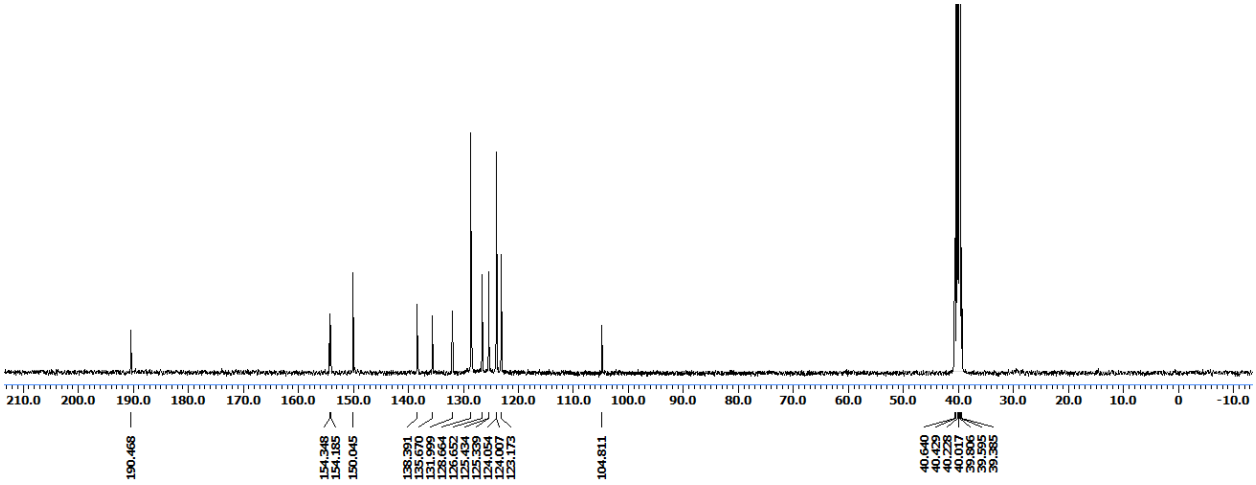


^{13}C NMR

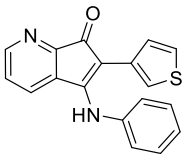


5-(Phenylamino)-6-(thiophen-3-yl)-7*H*-cyclopenta[b]pyridin-7-one (5e)





HRMS



5-(Phenylamino)-6-(thiophen-3-yl)-7*H*-cyclopenta[b]pyridin-7-one (5e)

Qualitative Compound Report

Data File	KMS-1114.d	**Sample Name**	KMS-1114
Sample Type	Sample	**Position**	P1-A1
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	06-06-2019 11:46:06
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

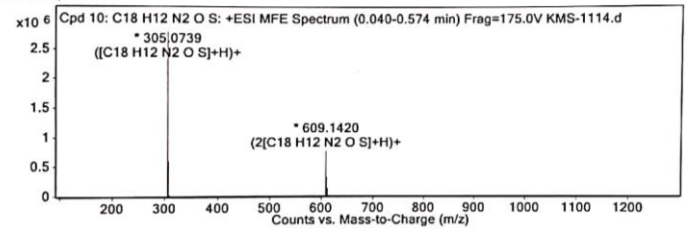
Sample Group **Info.**
Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

Compound Table

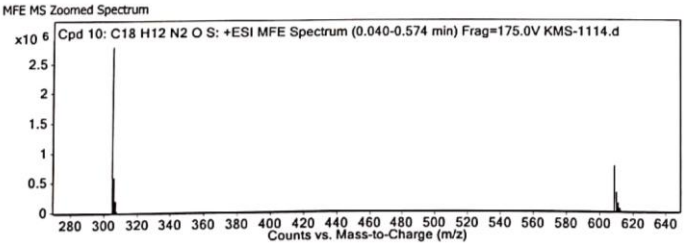
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 10: C18 H12 N2 O S	0.134	304.0665	C18 H12 N2 O S	C18 H12 N2 O S	1.66	C18 H12 N2 O S

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 10: C18 H12 N2 O S	305.0739	0.134	Find by Molecular Feature	304.0665

MFE MS Spectrum



MFE MS Zoomed Spectrum

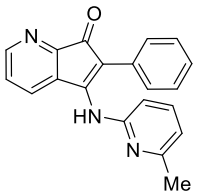


MS Spectrum Peak List

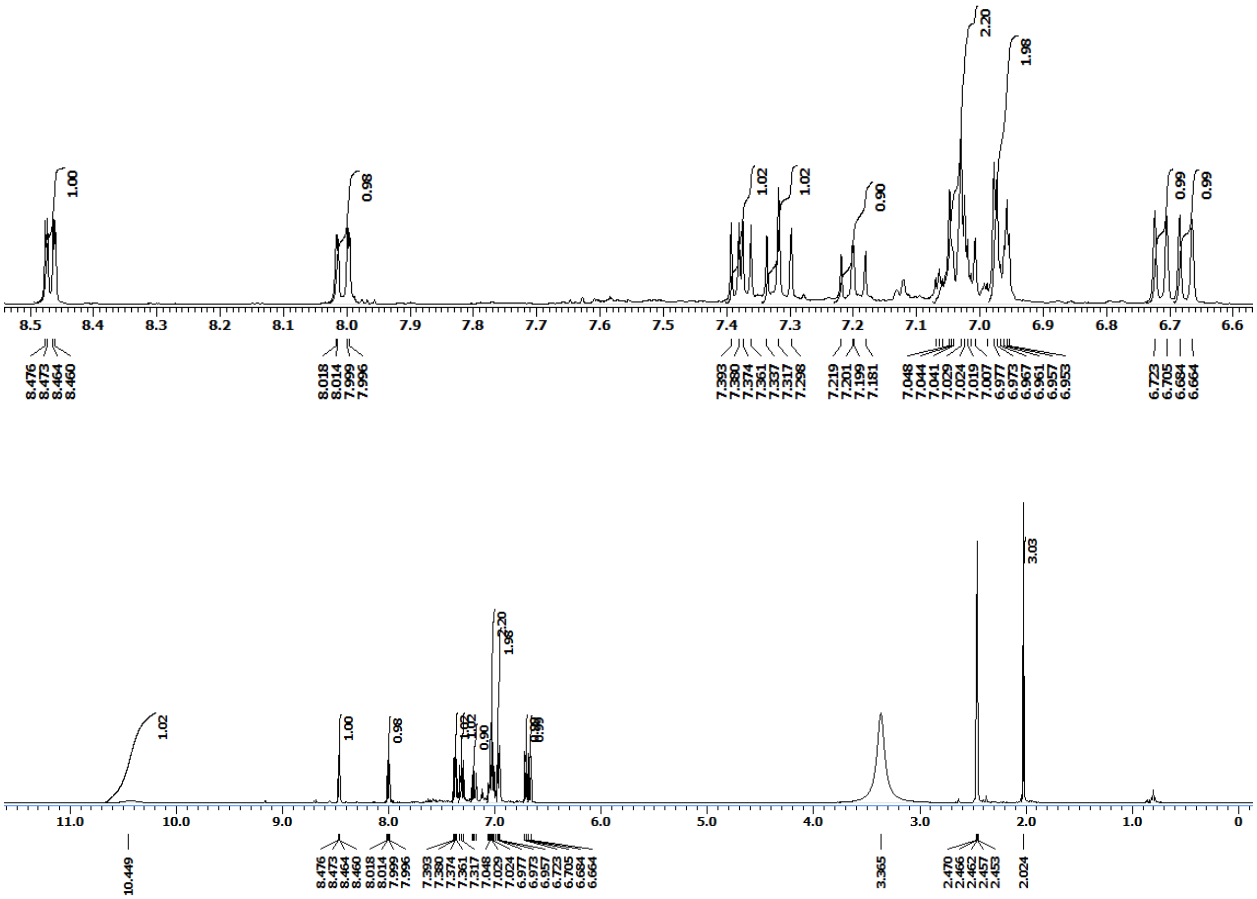
m/z	z	Abund	Formula	Ion
305.0739	1	2796885.25	C18 H12 N2 O S	(M+H)+
306.0758	1	592878.43	C18 H12 N2 O S	(M+H)+
307.0751	1	144864.79	C18 H12 N2 O S	(M+H)+
308.0741	1	23009.59	C18 H12 N2 O S	(M+H)+
309.076	1	1770.96	C18 H12 N2 O S	(M+H)+
609.142	1	765166.44	C18 H12 N2 O S	(2M+H)+
610.1429	1	322108.1	C18 H12 N2 O S	(2M+H)+
611.1406	1	127058.55	C18 H12 N2 O S	(2M+H)+
612.1403	1	34483.77	C18 H12 N2 O S	(2M+H)+
613.14	1	7929.1	C18 H12 N2 O S	(2M+H)+

--- End Of Report ---

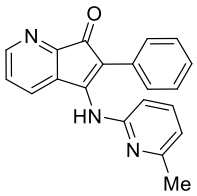
^{1}H NMR



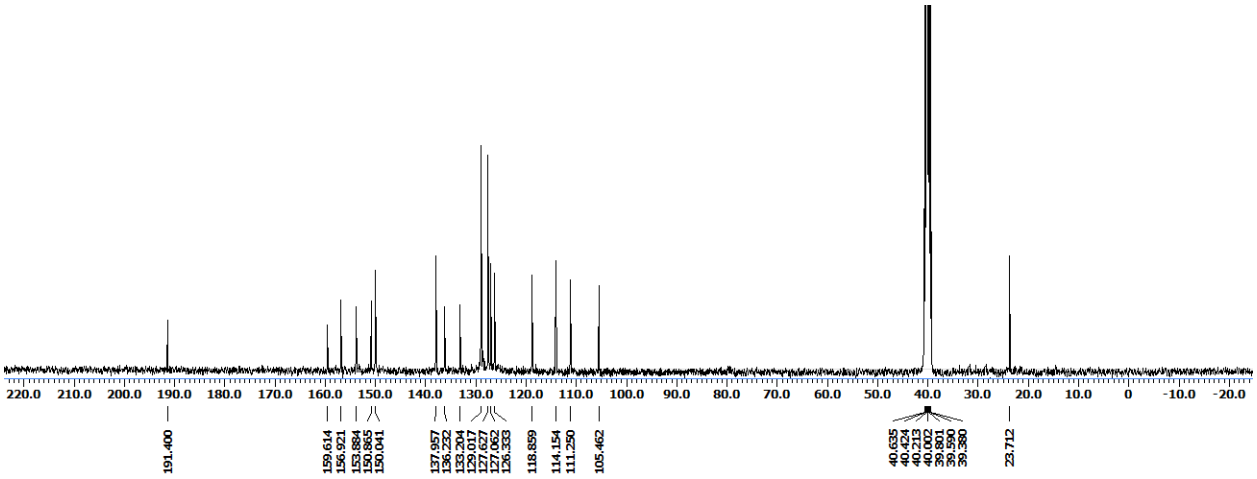
5-((6-Methylpyridin-2-yl)amino)-6-phenyl-7*H*-cyclopenta[b]pyridin-7-one (5f)



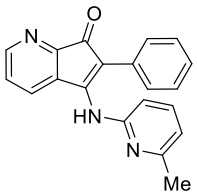
^{13}C NMR



5-((6-Methylpyridin-2-yl)amino)-6-phenyl-7*H*-cyclopenta[b]pyridin-7-one (5f)



HRMS



5-((6-Methylpyridin-2-yl)amino)-6-phenyl-7*H*-cyclopenta[b]pyridin-7-one (5f)

Qualitative Compound Report

Data File	KMS-1100.d	**Sample Name**	KMS-1100
Sample Type	Sample	**Position**	P1-C3
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	17-05-2019 12:35:11
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

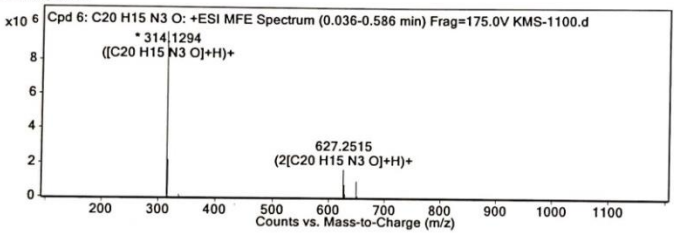
Sample Group **Info.**
Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

Compound Table

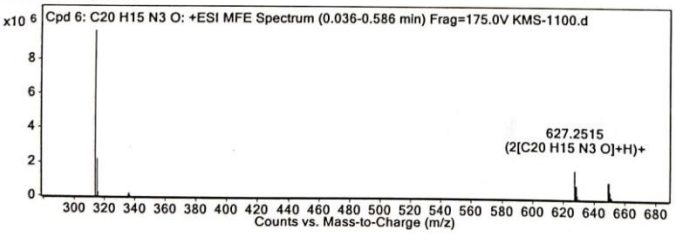
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 6: C20 H15 N3 O	0.093	313.1219	C20 H15 N3 O	C20 H15 N3 O	-1.28	C20 H15 N3 O

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 6: C20 H15 N3 O	314.1294	0.093	Find by Molecular Feature	313.1219

MFE MS Spectrum



MFE MS Zoomed Spectrum

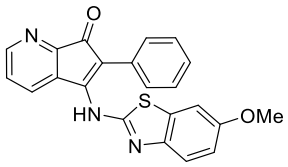


MS Spectrum Peak List

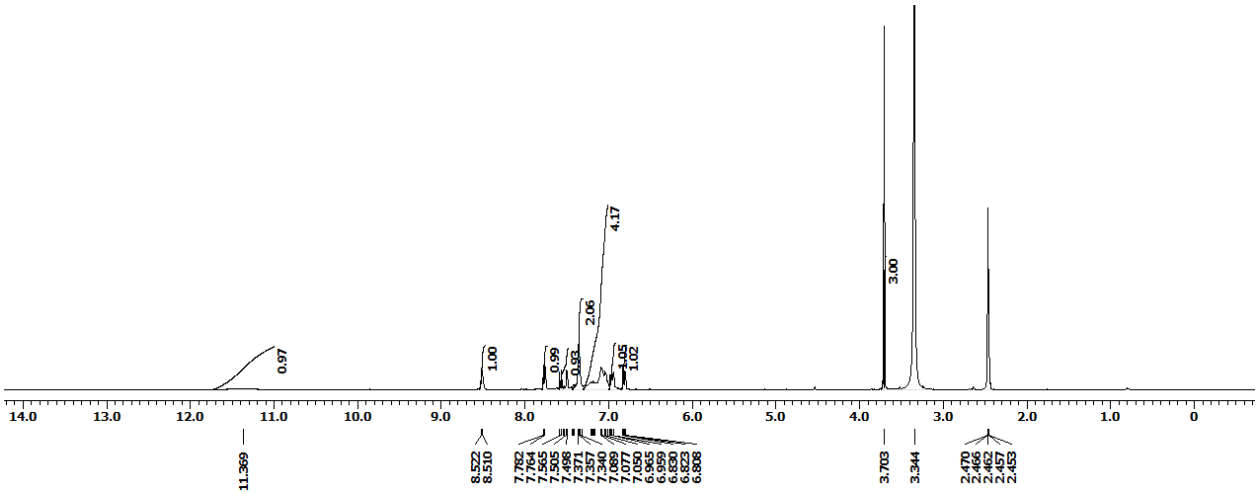
m/z	z	Abund	Formula	Ion
314.1294	1	9614402	C20 H15 N3 O	(M+H)+
315.1328	1	2168715.06	C20 H15 N3 O	(M+H)+
316.1361	1	269489.08	C20 H15 N3 O	(M+H)+
336.1112	1	163392.58	C20 H15 N3 O	(M+Na)+
627.2515	1	1659206.63	C20 H15 N3 O	(2M+H)+
628.2546	1	756310.06	C20 H15 N3 O	(2M+H)+
629.2574	1	173590.29	C20 H15 N3 O	(2M+H)+
649.2333	1	944545.44	C20 H15 N3 O	(2M+Na)+
650.2362	1	425857.38	C20 H15 N3 O	(2M+Na)+
651.2389	1	95747.09	C20 H15 N3 O	(2M+Na)+

--- End Of Report ---

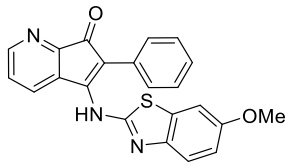
^{1}H NMR



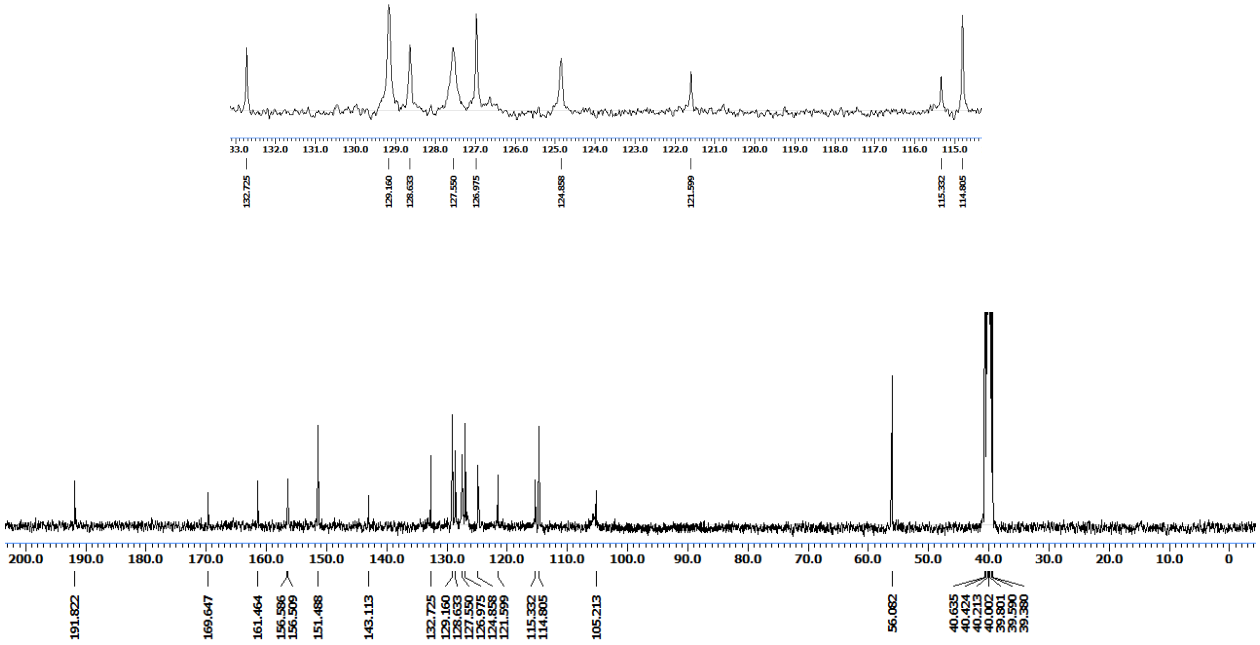
5-((6-Methoxybenzo[d]thiazol-2-yl)amino)-6-phenyl-7*H*-cyclopenta[b]pyridin-7-one (5g)



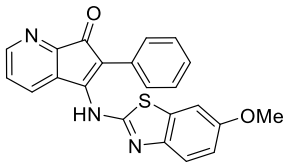
^{13}C NMR



5-((6-Methoxybenzo[d]thiazol-2-yl)amino)-6-phenyl-7*H*-cyclopenta[b]pyridin-7-one (5g)



HRMS



5-((6-Methoxybenzo[d]thiazol-2-yl)amino)-6-phenyl-7*H*-cyclopenta[b]pyridin-7-one (5g)

Qualitative Compound Report

Data File	KMS-1108.d	**Sample Name**	KMS-1108
Sample Type	Sample	**Position**	P1-A2
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	29-05-2019 12:51:55
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

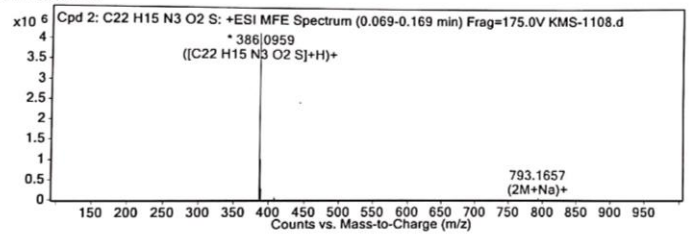
Sample Group **Info.**
Acquisition SW 6200 series TOF/6500 series
Version Q-TOF B.05.01 (B5125.1)

Compound Table

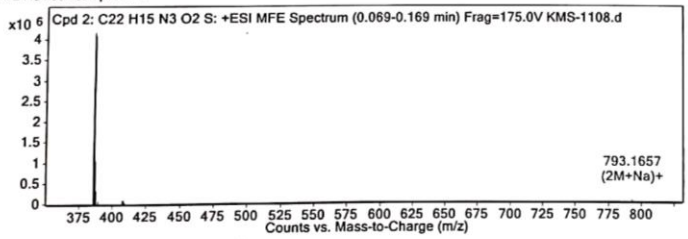
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 2: C22 H15 N3 O2 S	0.094	385.0887	C22 H15 N3 O2 S	C22 H15 N3 O2 S	-0.6	C22 H15 N3 O2 S

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 2: C22 H15 N3 O2 S	386.0959	0.094	Find by Molecular Feature	385.0887

MFE MS Spectrum



MFE MS Zoomed Spectrum

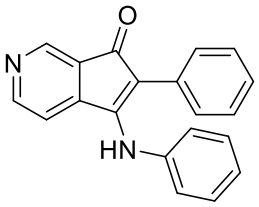


MS Spectrum Peak List

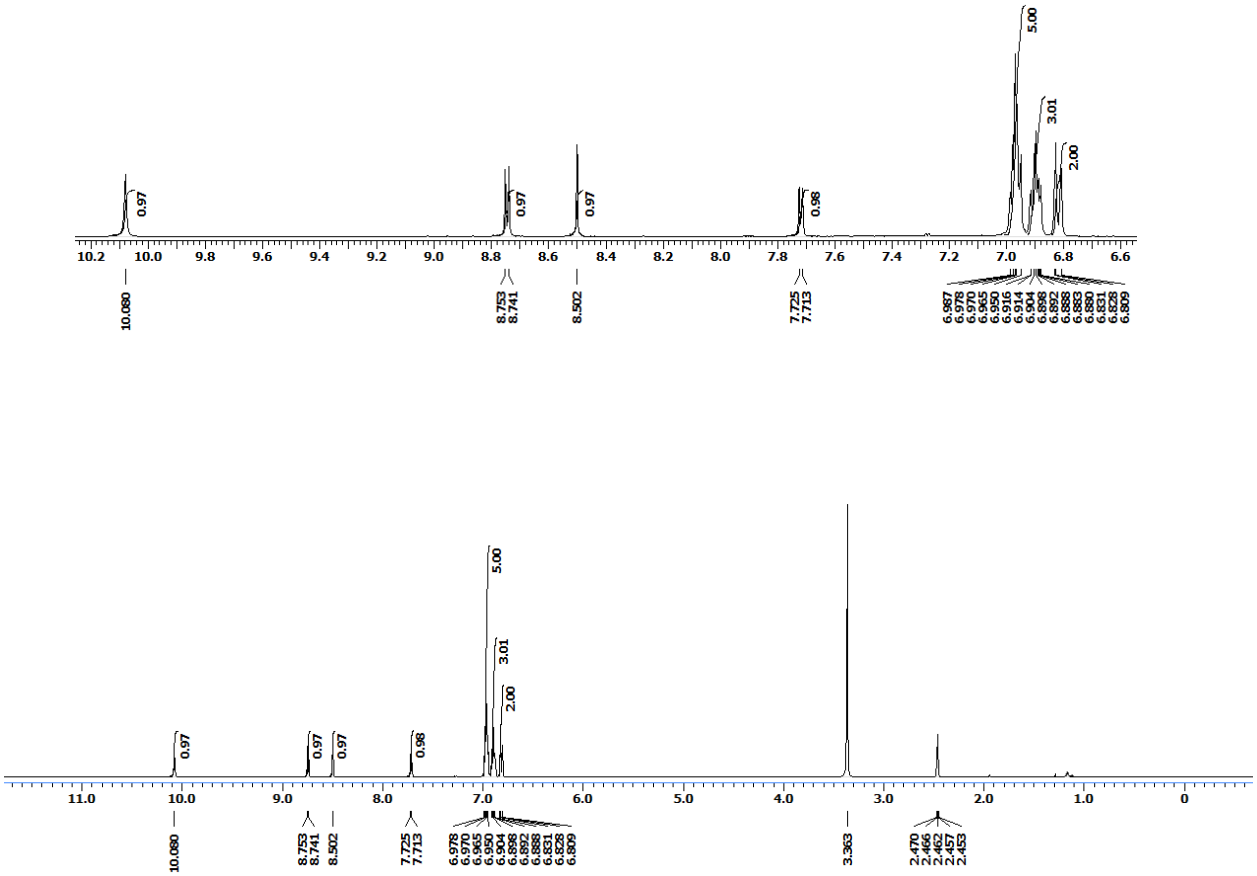
m/z	z	Abund	Formula	Ion
386.0959	1	4177982	C22 H15 N3 O2 S	(M+H)+
387.0993	1	1003304.32	C22 H15 N3 O2 S	(M+H)+
388.0967	1	285319.42	C22 H15 N3 O2 S	(M+H)+
389.097	1	36592.01	C22 H15 N3 O2 S	(M+H)+
390.0995	1	10181.96	C22 H15 N3 O2 S	(M+H)+
408.0775	1	62033.03	C22 H15 N3 O2 S	(M+Na)+
409.0804	1	17645.63	C22 H15 N3 O2 S	(M+Na)+
793.1657	1	33034.07		(2M+Na)+
794.1692	1	17053.59		(2M+Na)+
795.1682	1	8480.13		(2M+Na)+

--- End Of Report ---

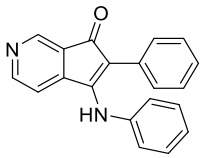
^{1}H NMR



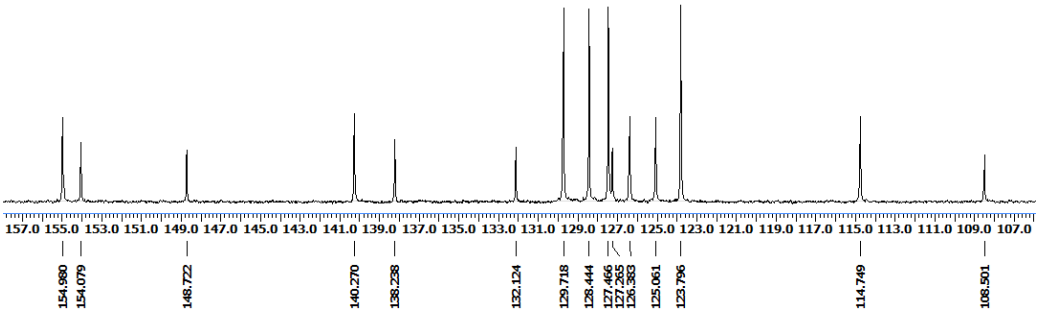
6-Phenyl-5-(phenylamino)-7*H*-cyclopenta[c]pyridin-7-one (7a)

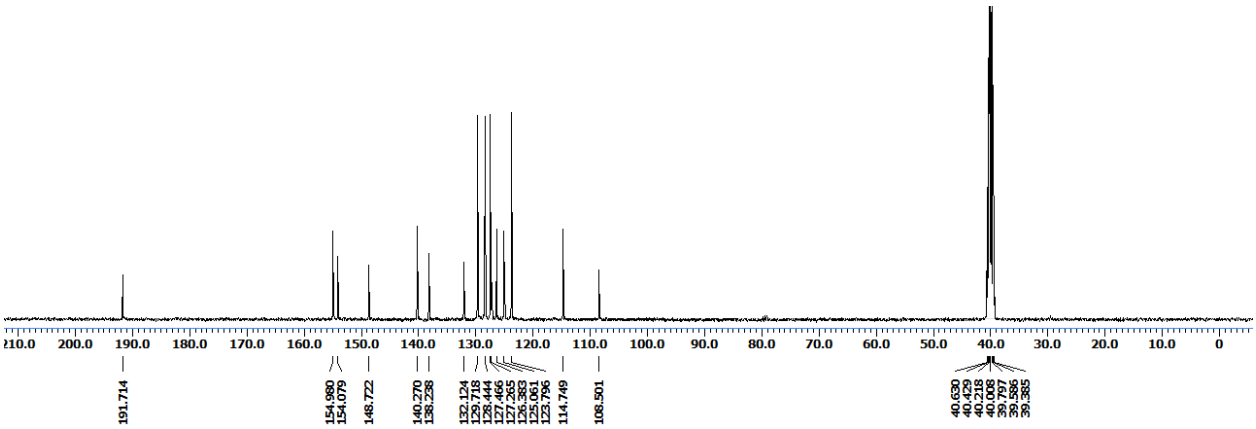


^{13}C NMR

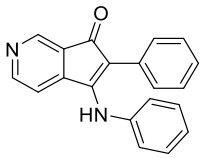


6-Phenyl-5-(phenylamino)-7*H*-cyclopenta[c]pyridin-7-one (7a)





HRMS



6-Phenyl-5-(phenylamino)-7*H*-cyclopenta[c]pyridin-7-one (7a)

Qualitative Compound Report

Data File	KMS-1125.d	**Sample Name**	KMS-1125
Sample Type	Sample	**Position**	P1-A3
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	19-06-2019 12:31:53
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

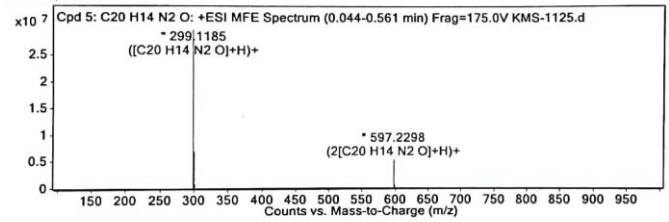
Sample Group **Info.**
Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

Compound Table

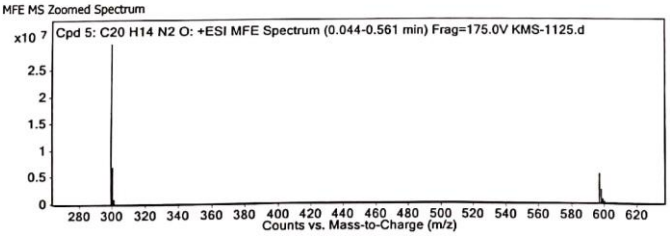
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 5: C20 H14 N2 O	0.108	298.1114	C20 H14 N2 O	C20 H14 N2 O	-2.53	C20 H14 N2 O

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 5: C20 H14 N2 O	299.1185	0.108	Find by Molecular Feature	298.1114

MFE MS Spectrum



MFE MS Zoomed Spectrum

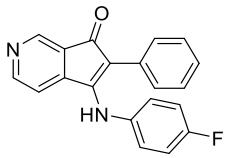


MS Spectrum Peak List

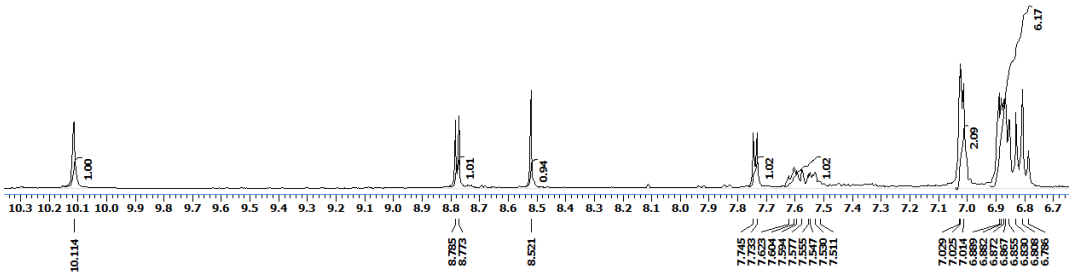
m/z	z	Abund	Formula	Ion
299.1185	1	29818084	C20 H14 N2 O	(M+H)+
300.1223	1	6980677.04	C20 H14 N2 O	(M+H)+
301.1262	1	720107.61	C20 H14 N2 O	(M+H)+
302.1295	1	55379.51	C20 H14 N2 O	(M+H)+
303.1296	1	7560.1	C20 H14 N2 O	(M+H)+
597.2298	1	5346137	C20 H14 N2 O	(2M+H)+
598.2333	1	2409423.37	C20 H14 N2 O	(2M+H)+
599.2358	1	557798.93	C20 H14 N2 O	(2M+H)+
600.236	1	88744.43	C20 H14 N2 O	(2M+H)+
601.2303	1	16575.13	C20 H14 N2 O	(2M+H)+

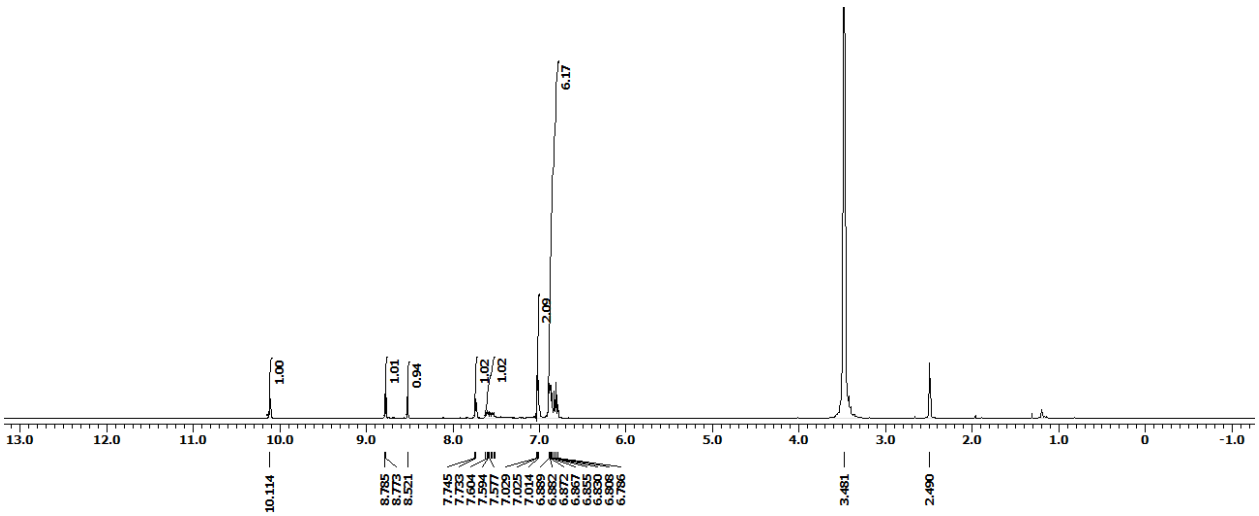
— End Of Report —

^{1}H NMR

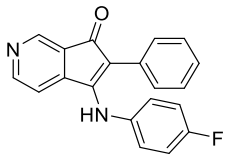


5-((4-Fluorophenyl)amino)-6-phenyl-7*H*-cyclopenta[c]pyridin-7-one (7b)

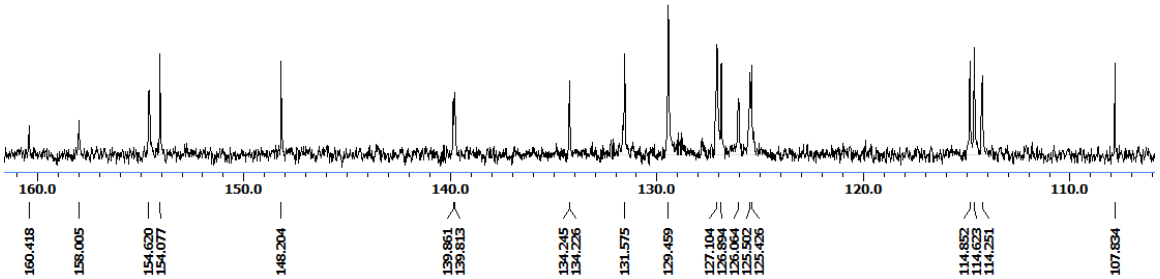


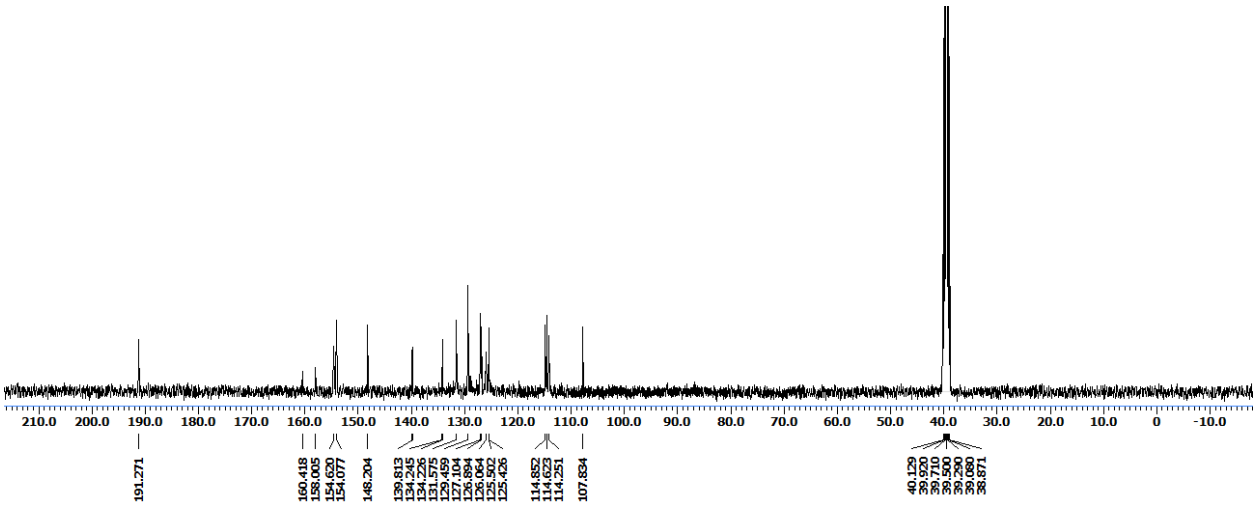


^{13}C NMR

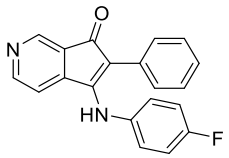


5-((4-Fluorophenyl)amino)-6-phenyl-7*H*-cyclopenta[c]pyridin-7-one (7b)

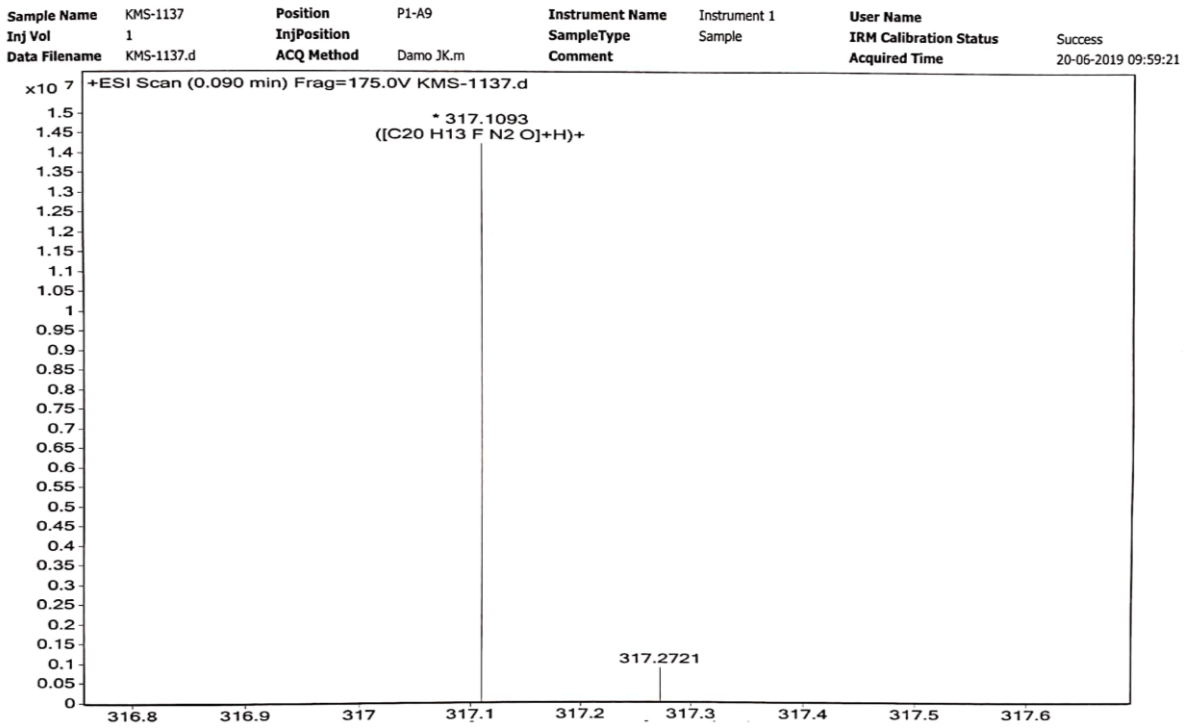




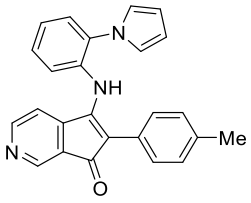
HRMS



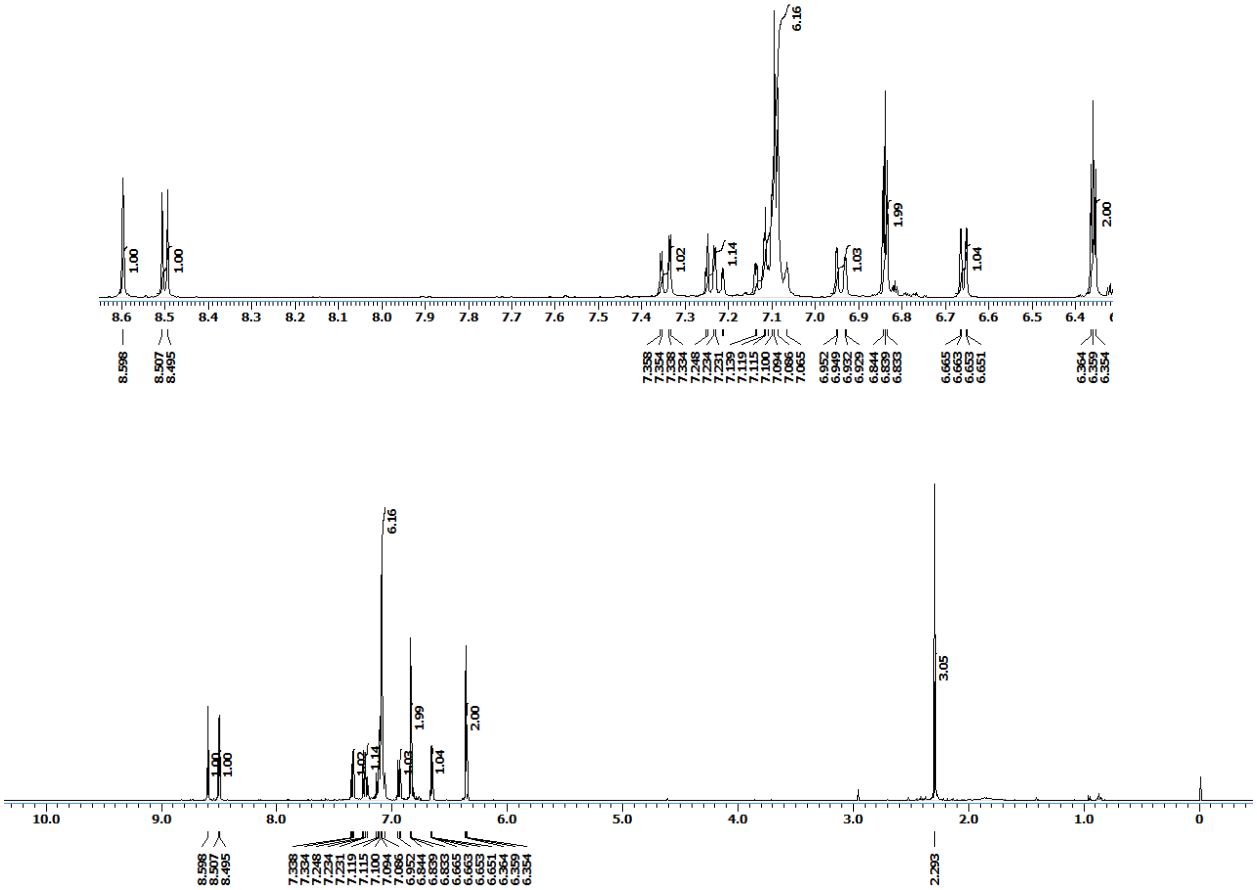
5-((4-Fluorophenyl)amino)-6-phenyl-7*H*-cyclopenta[c]pyridin-7-one (7b)



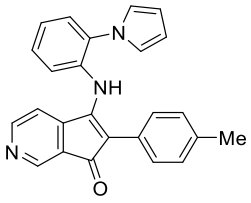
^{1}H NMR



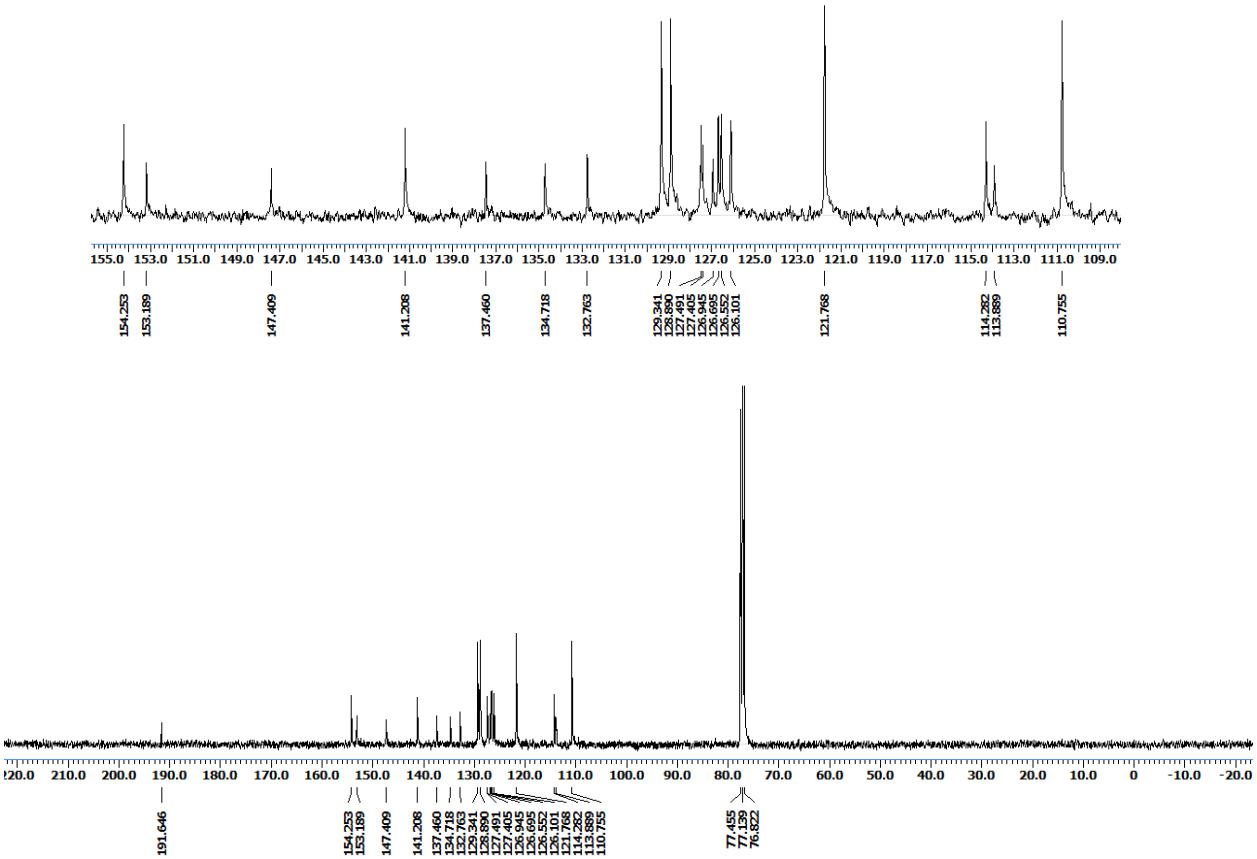
5-((2-(1*H*-pyrrol-1-yl)phenyl)amino)-6-(*p*-tolyl)-7*H*-cyclopenta[c]pyridin-7-one (7c)



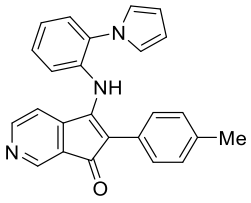
^{13}C NMR



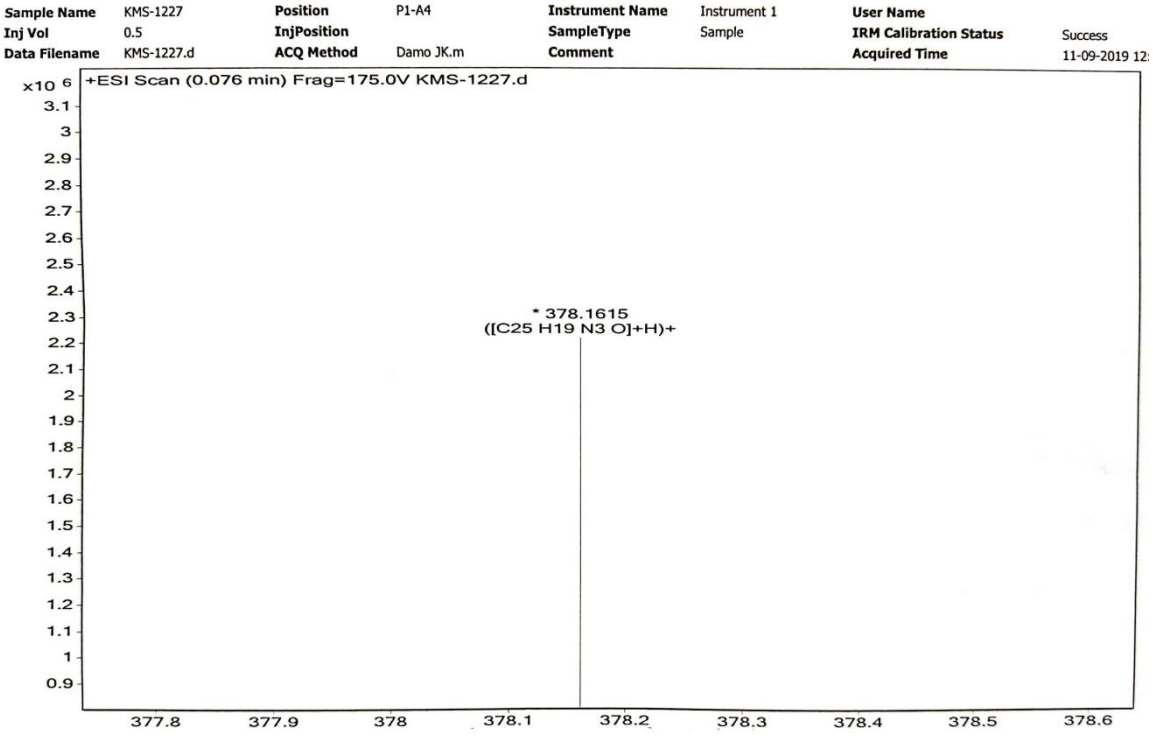
5-((2-(1*H*-pyrrol-1-yl)phenyl)amino)-6-(*p*-tolyl)-7*H*-cyclopenta[c]pyridin-7-one (7c)



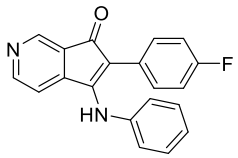
HRMS



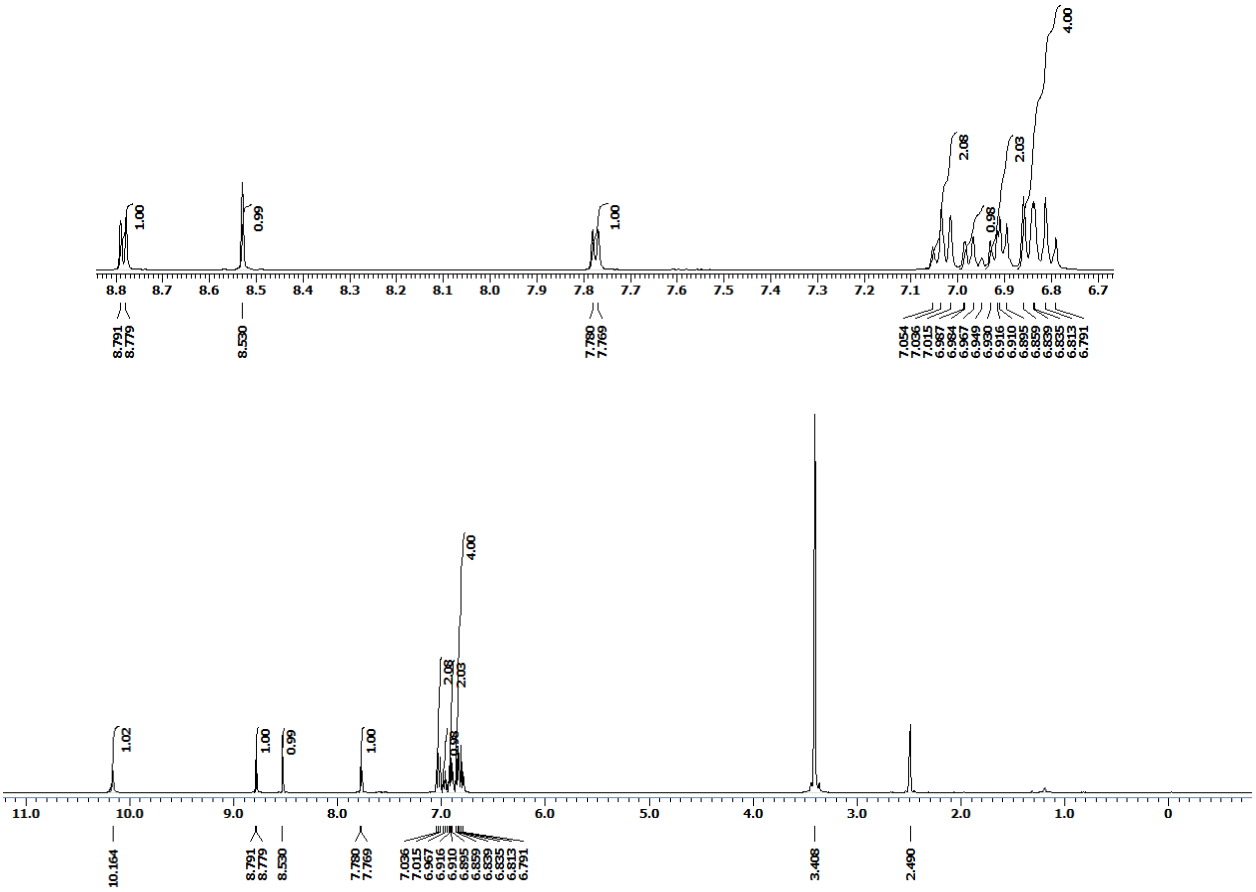
5-((2-(1*H*-pyrrol-1-yl)phenyl)amino)-6-(*p*-tolyl)-7*H*-cyclopenta[c]pyridin-7-one (7c)



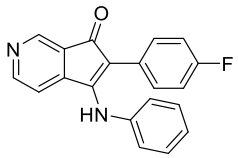
^{1}H NMR



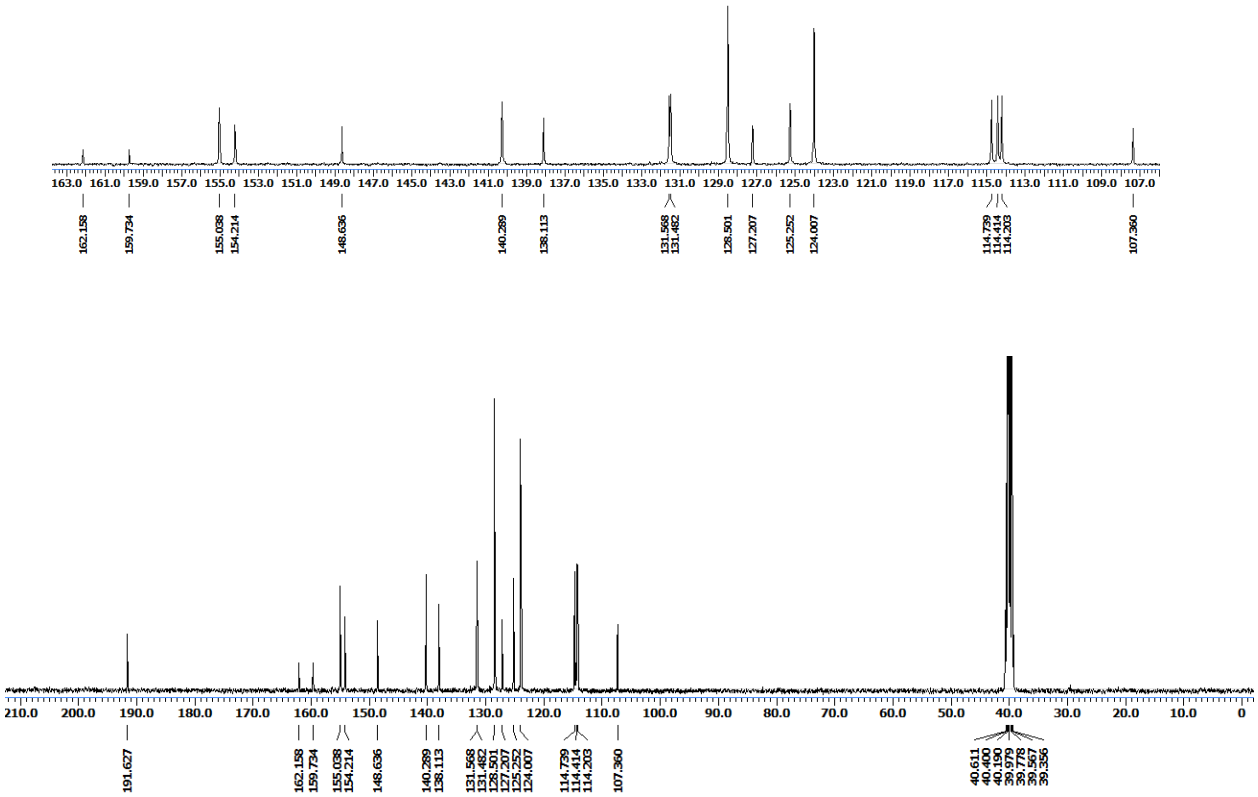
6-(4-Fluorophenyl)-5-(phenylamino)-7*H*-cyclopenta[c]pyridin-7-one (7d)



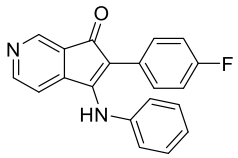
^{13}C NMR



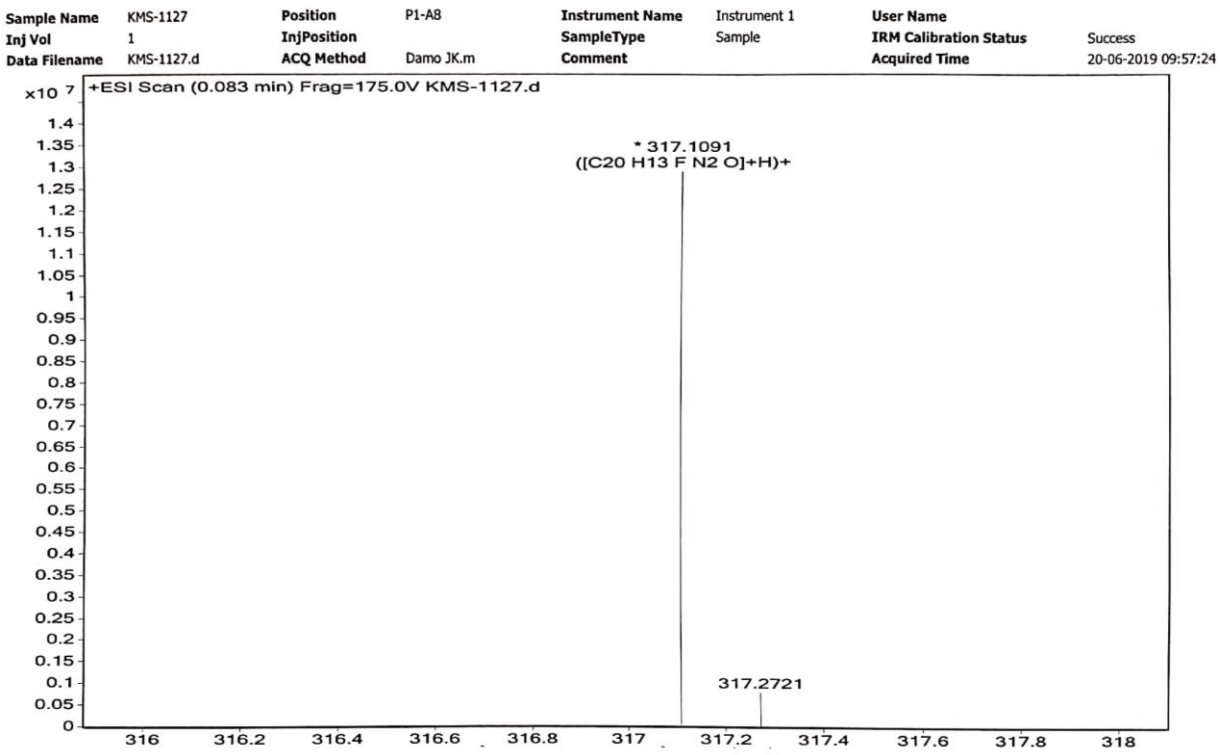
6-(4-Fluorophenyl)-5-(phenylamino)-7*H*-cyclopenta[c]pyridin-7-one (7d)



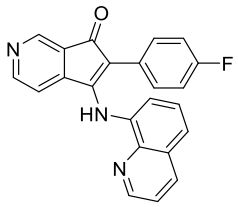
HRMS



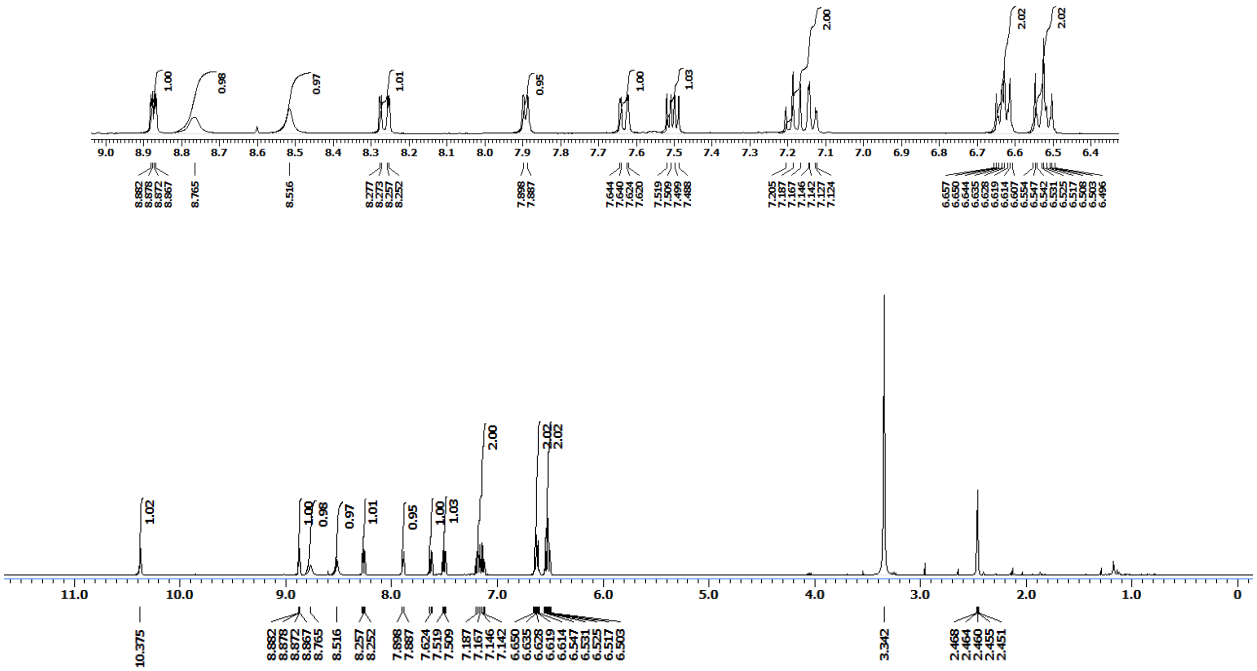
6-(4-Fluorophenyl)-5-(phenylamino)-7*H*-cyclopenta[c]pyridin-7-one (7d)



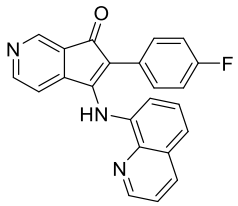
^{1}H NMR



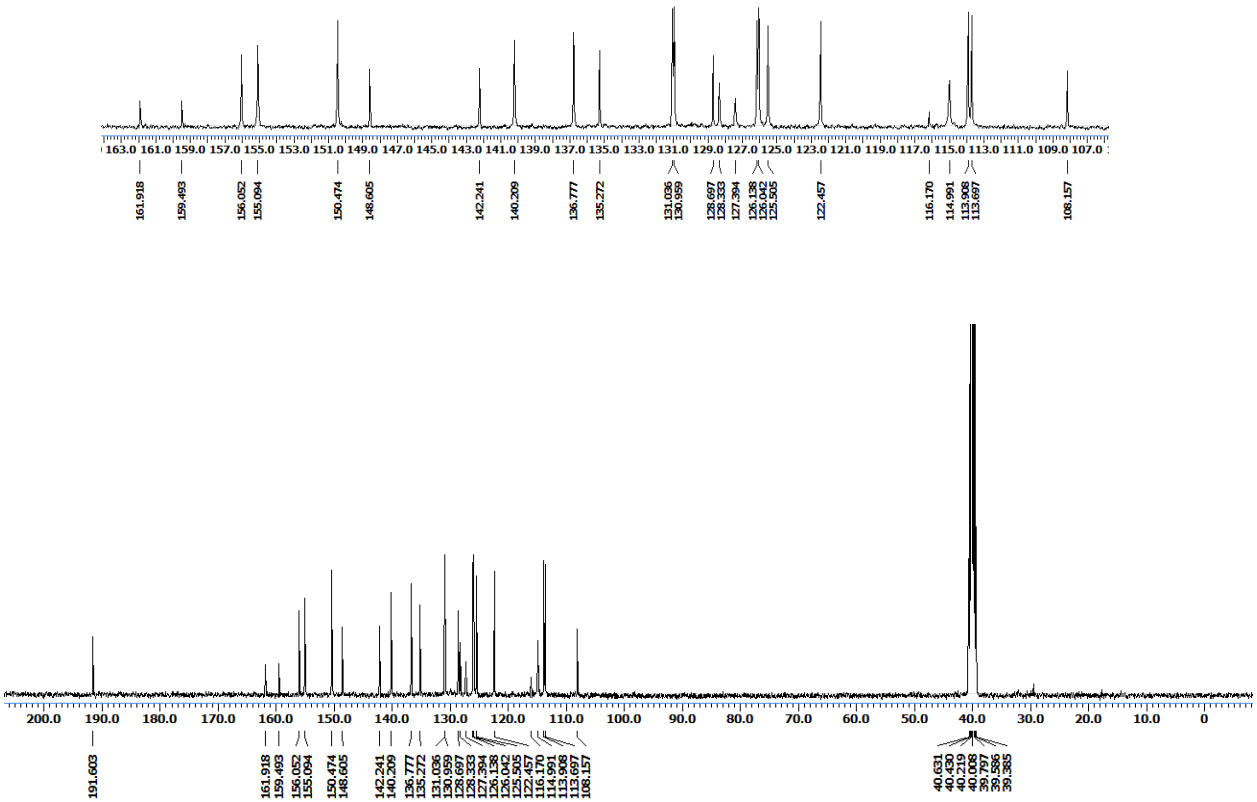
6-(4-Fluorophenyl)-5-(quinolin-8-ylamino)-7*H*-cyclopenta[c]pyridin-7-one (7e)



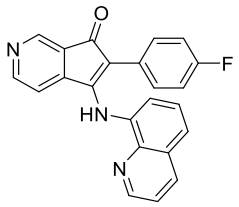
^{13}C NMR



6-(4-Fluorophenyl)-5-(quinolin-8-ylamino)-7*H*-cyclopenta[c]pyridin-7-one (7e)



HRMS



6-(4-Fluorophenyl)-5-(quinolin-8-ylamino)-7*H*-cyclopenta[c]pyridin-7-one (7e)

Qualitative Compound Report

Data File	KMS-1145.d	**Sample Name**	KMS-1145
Sample Type	Sample	**Position**	P1-A3
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	24-06-2019 12:34:41
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

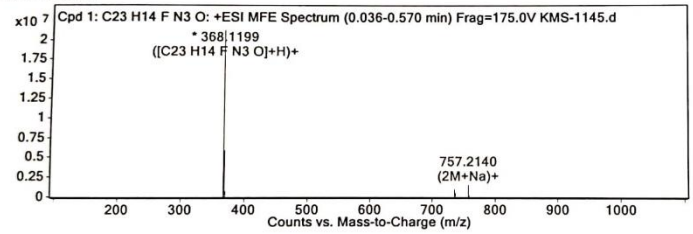
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)

Compound Table

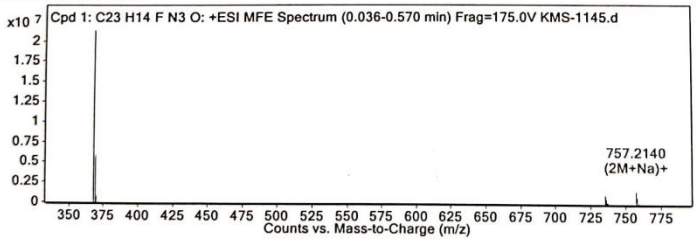
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 1: C23 H14 F N3 O	0.094	367.1123	C23 H14 F N3 O	C23 H14 F N3 O	-0.68	C23 H14 F N3 O

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C23 H14 F N3 O	368.1199	0.094	Find by Molecular Feature	367.1123

MFE MS Spectrum



MFE MS Zoomed Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
368.1199	1	21284092	C23 H14 F N3 O	(M+H)+
369.1233	1	5885643.83	C23 H14 F N3 O	(M+H)+
370.1264	1	805301.23	C23 H14 F N3 O	(M+H)+
371.1293	1	72197.84	C23 H14 F N3 O	(M+H)+
735.2318	1	1032817.75	C23 H14 F N3 O	(2M+H)+
736.2348	1	535410.01	C23 H14 F N3 O	(2M+H)+
737.2375	1	134605.75	C23 H14 F N3 O	(2M+H)+
757.214	1	1533683.88		(2M+Na)+
758.2173	1	800732.34		(2M+Na)+
759.2197	1	200430.81		(2M+Na)+

--- End Of Report ---